Furneaux, A. G., Piro, N. A., Hernández Sánchez, R., Gramigna, K. M., Fey, N., Robinson, M. J., Kassel, W. S., & Nataro, C. (2016). Spectroscopic, structural and computational analysis of $[Re(CO)_3(dippM)Br]^{n+}$ (dippM = 1,1′-bis(diiso-propylphosphino)metallocene, M = Fe, n = 0 or 1; M = Co, n = 1). *Dalton Transactions*, *45*(11), 4819-4827. https://doi.org/10.1039/c5dt04721h

Peer reviewed version

Link to published version (if available):
10.1039/c5dt04721h

Spectroscopic, structural and computational analysis of $[Re(CO)_3(dippM)Br]^{n+}$ (dippM = 1,1′-bis(diiso-propylphosphino)metallocene, M = Fe, n = 0 or 1; M = Co, n = 1)

Aliza G. Furneaux, Nicholas A. Piro, Raúl Hernández Sánchez, Kathryn M. Gramigna, Natalie Fey, Michael J. Robinson, W. Scott Kassel, and Chip Nataro

Supporting Information

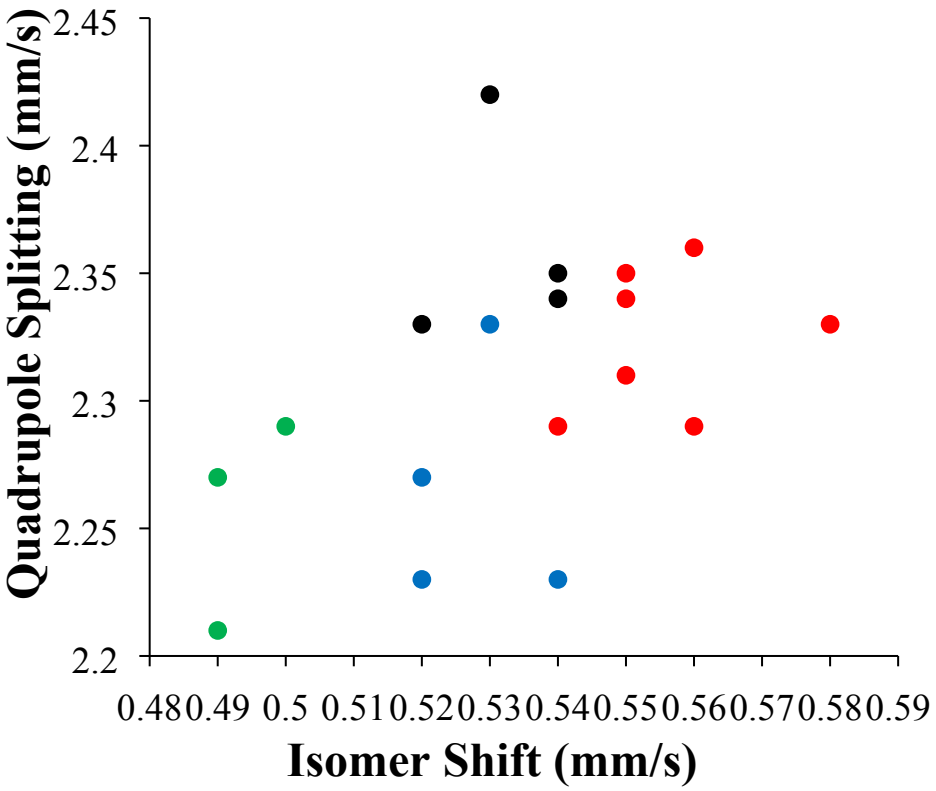


Fig. S1 ^{57}Fe Mössbauer data (quadrupole splitting vs. isomer shift) for ferrocene and 1,1′-bis(phosphino)ferrocene ligands (•) and coordinated 1,1′-bis(phosphino)ferrocene ligands in compounds with square planar (•), octahedral (•) and tetrahedral (•) geometries. Adopted from figures in references 1 and 2.

Table 1 ^{57}Fe Mössbauer data presented in Fig. S1

Compound	Quadrupole splitting (mm/s)	Isomer shift (mm/s)	Ref
ferrocene	0.53	2.42	3
dppf	0.52	2.33	3
dippf	0.54	2.34	This work
dtbpf	0.54	2.35	4
$Co(dppf)Cl_2$	0.55	2.34	2
$Ni(dppf)Cl_2$	0.54	2.29	2
$Zn(dppf)Cl_2$	0.55	2.35	3
$Hg(dppf)Cl_2$	0.56	2.36	3
$Fe(dppf)Cl_2$	0.56	2.29	2
$Ni(dppf)Br_2$	0.55	2.31	2
$Ni(dppf)I_2$	0.58	2.33	2
$Pd(dppf)Cl_2$	0.49	2.21	2
$Pt(dppf)Cl_2$	0.5	2.29	3
$Pd(dtbpf)Cl_2$	0.49	2.27	4
$Cr(dppf)(CO)_4$	0.52	2.23	2
$Mo(dppf)(CO)_4$	0.52	2.27	2
$W(dppf)(CO)_4$	0.54	2.23	2
$Re(CO)_3(dippf)Br$	0.53	2.33	This work

Fig. S2 Plot of spin density for $[dippf]^+$ at the UB3LYP level of theory, shown as an isosurface of 0.0004 au. The Mulliken spin density shows >98 % on the $FeCp_2$ unit, with >78 % on Fe alone.

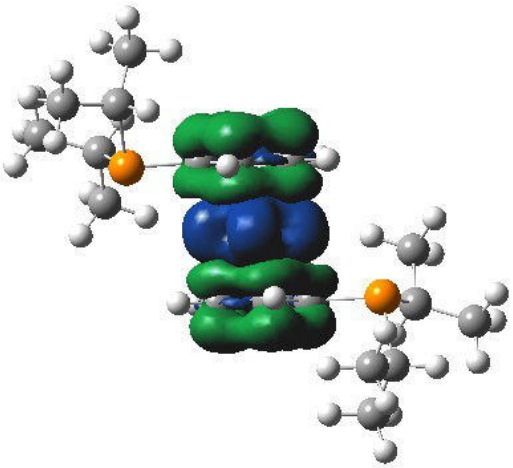


Fig. S3. IR spectrum of $[Re(CO)_3(dippf)Br][BF_4]$ in methylene chloride.

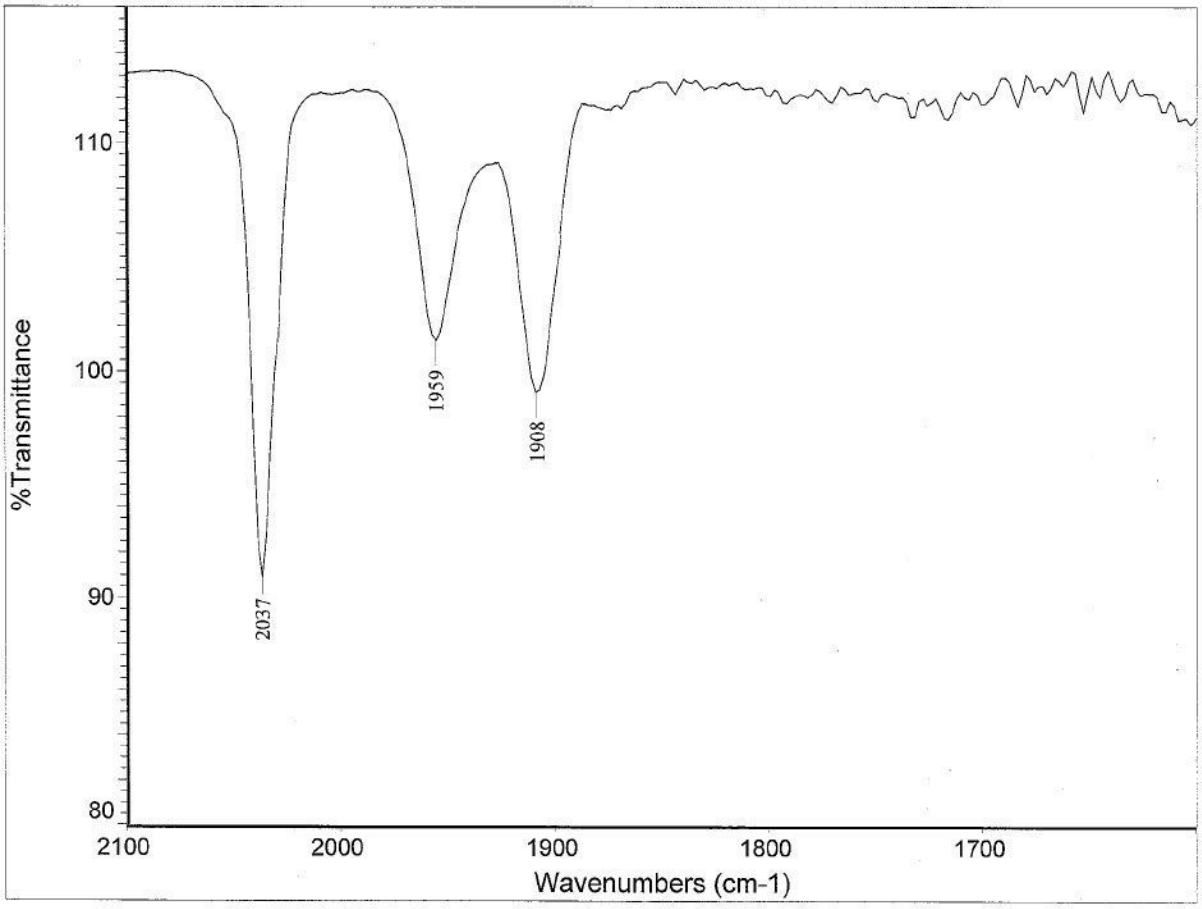


Fig. S4. IR spectrum of acetylferrocene in methylene chloride.

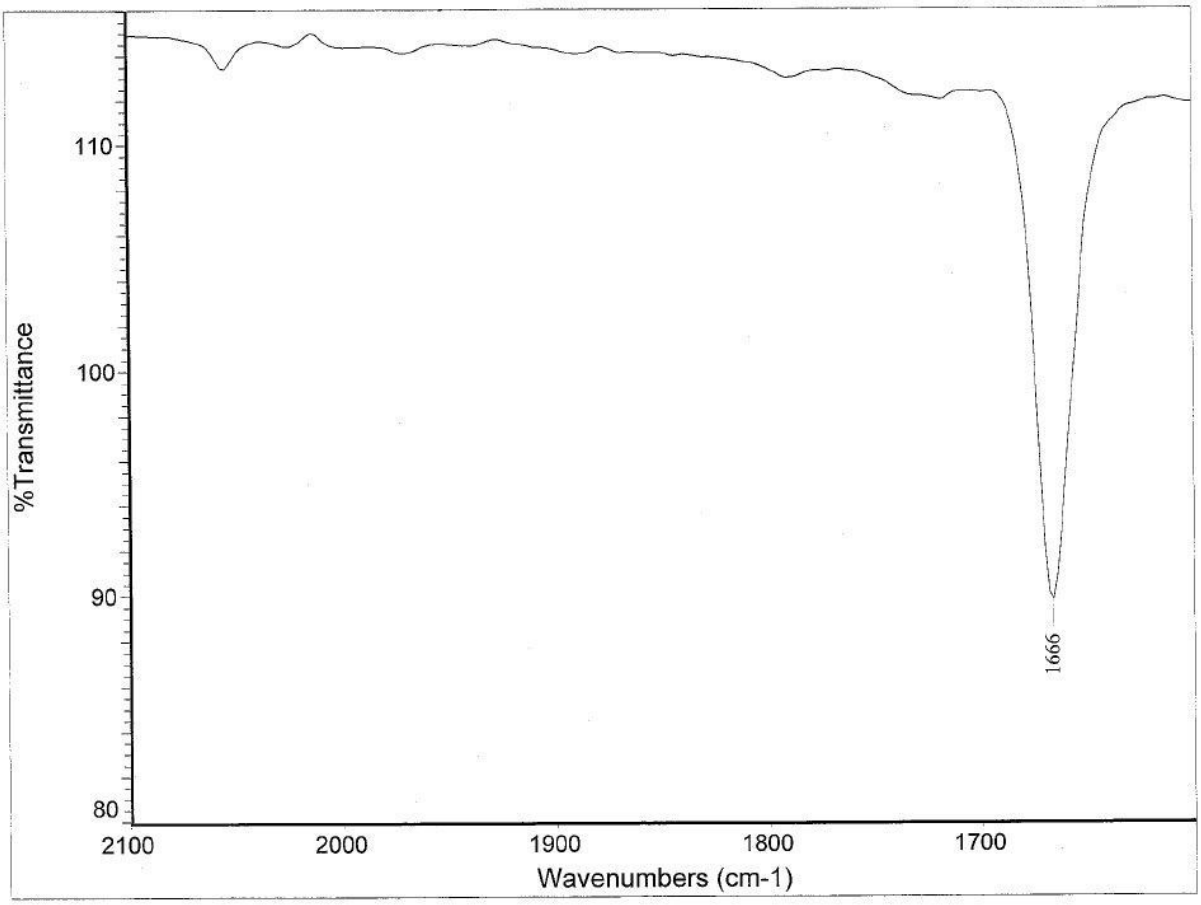
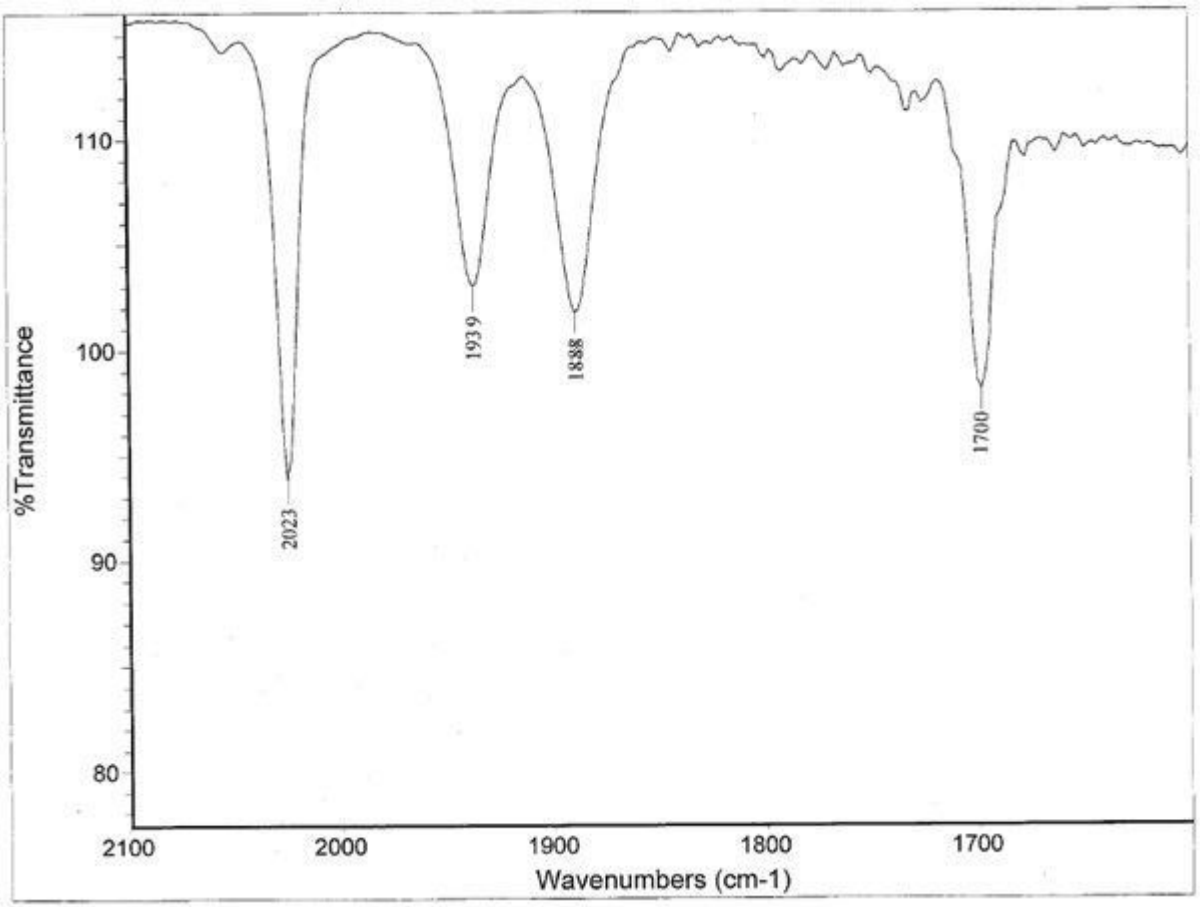


Fig. S5. IR spectrum of the reaction of $[Re(CO)_3(dippf)Br][BF_4]$ with acetylferrocene in methylene chloride.



Computational Details

Unless stated otherwise, structures discussed here were optimized in Jaguar[5] with the standard B3LYP[6] density functional as implemented and all calculations were run as unrestricted (UB3LYP); trial calculations with spin-restricted open shell DFT (ROB3LYP) repeatedly failed to converge, especially for the doublet metallocenium configurations. The Jaguar triple-ζ form of the standard Los Alamos ECP basis set (LACV3P*) was used on the transition metal atoms, employing the 6-311G* basis for all other atoms with five spherical harmonic components of the polarization functions. "Loose" convergence (5 times larger than default criteria) was used for geometry optimizations and calculations were performed on isolated molecules. All lowest energy conformations were confirmed as minima by frequency calculations at this level of theory, also allowing derivation of gas-phase thermodynamic corrections. In addition, solvation corrections were calculated as single point energies with the Poisson Boltzmann Finite (PBF) continuum-dielectric solvation model as implemented in Jaguar, using dichloromethane as the solvent.[7]

Structures were re-optimized in Gaussian,[8] using the spin-unrestricted standard density functional UB3LYP[6a-f] as implemented. Calculations generally used the standard 6-311+G** basis set, but with only the five spherical harmonic components of the polarization functions, on all atoms apart from rhenium, and iron, where the corresponding Stuttgart relativistic ECP basis set[9] was used to describe 60 and 10 core electrons respectively. For the two Re/dippf complexes, full convergence could only be achieved with the smaller 6-31G* basis set on the non-metal atoms. As we were using the unrestricted open shell approach for all calculations, stability tests of the wavefunction as implemented in Gaussian were carried out and, where a wavefunction instability was detected and corrected by this approach (keyword stable=opt), the resulting guess function was used as input for further geometry optimisation. Vibrational frequencies were calculated at the same level of theory, in some cases with tighter convergence criteria to address low negative frequencies (keywords opt=(tight) Int=(Grid=Ultrafine) CPHF=(Grid=Fine)), allowing the determination of zero-point energies and gas-phase thermodynamic corrections (298 K), as well as confirmation that all structures reported here are true minima. Solvation effects were considered by single point calculations on the gas-phase optimised geometries using a continuum dielectric field; the Integral Equation Formalism Polarizable Continuum Model (IEF-PCM) continuum dielectric solvation model[10] was used with dichloromethane as the solvent. These were not corrected for solvation free energy effects.

Input geometries of the rhenium complexes were taken from available x-ray structural data as reported here, which sampled several conformations for the *iso*-propyl substituents as shown in the structural data below; the metallocene metal as well as complex charge and multiplicity were modified to generate starting geometries from these. For the ligands, rhenium atoms were removed from these complexes and different conformations with respect to the cyclopentadienyl substituents were generated by ring rotation, and the graphical user interface of the relevant software package was used to generate unsubstituted metallocene structures, both with and without symmetry; the results reported here do not have symmetry.

Summary of Calculated Structural Data

Table 2 Jaguar calculated (UB3LYP/6-311G*, LACV3P* on Re, Fe, Br) ligands and metallocenes for comparison

	$[Re(CO)_3(dippf)Br]$ from XRD	**$[Re(CO)_3(dippf)Br]$ from Fe(III) XRD**	**$[Re(CO)_3(dippf)Br]^+$ from XRD**
rel. E (gas phase, same M, kcal mol^{-1})	0.83	0.00	145.52
C-O (trans to P)	1.150, 1.150	1.149, 1.150	1.145, 1.145
C-O (trans to Br)	1.161	1.162	1.157
Re-C (trans to P)	1.943, 1.945	1.943, 1.946	1.948, 1.952
Re-C (trans to Br)	1.907	1.905	1.913
Re-Br	2.758	2.762	2.751
Re-P	2.626, 2.647	2.611, 2.642	2.604, 2.637
M-X	1.680, 1.681	1.677, 1.678	1.739, 1.739
Re-C-O (trans to P)	175.1, 178.1	175.7, 178.0	175.4, 177.7
Re-C-O (trans to Br)	176.1	176.2	175.7
P-Re-P	100.0	94.8	98.4
Br-Re-P	85.3, 90.3	88.0, 89.8	87.7, 89.8
X_A-M-X_B	176.9	175.1	176.7
τ^a	-35.3	-2.3	-2.2
θ^b	3.16	5.41	8.02
$\delta_P{}^c$	-0.104	-0.168	-0.058
H-C-P-$C_{ring}{}^d$	132.7, 62.8; -47.7, 178.4	-52.7, -44.3; -41.1, 173.1	-54.0, -45.4; -41.4, 174.5

[a]The torsion angle C_A-X_A-X_B-C_B where C is the carbon atom bonded to phosphorus and X is the centroid. [b]The dihedral angle between the two C_5 rings. [c]Deviation of the P atom from the C_5 plane; a positive value means the P is closer to the Fe. [d]The torsion angle where H is the methyne hydrogen atom and the second C is the carbon atom of the C_5 ring bonded to the P atom.

	$[Re(CO)_3(dippc)Br]$ from Fe(III) XRD	**$[Re(CO)_3(dippc)Br]$ from Co(III) XRD**	**$[Re(CO)_3(dippc)Br]^+$ from XRD**
rel. E (gas phase, same M, kcal mol^{-1})	0.00	0.12	131.17
C-O (trans to P)	1.150, 1.150	1.150, 1.150	1.145, 1.146
C-O (trans to Br)	1.162	1.162	1.157
Re-C (trans to P)	1.942, 1.944	1.942, 1.945	1.949, 1.953
Re-C (trans to Br)	1.905	1.906	1.911
Re-Br	2.761	2.760	2.756
Re-P	2.621, 2.654	2.621, 2.656	2.586, 2.623
M-X	1.764, 1.767	1.764, 1.768	1.675, 1.675
Re-C-O (trans to P)	175.0, 177.3	175.0, 177.4	175.8, 178.3
Re-C-O (trans to Br)	174.9	175.0	175.7
P-Re-P	96.3	96.4	96.3
Br-Re-P	88.2, 89.6	88.2, 96.4	87.9, 89.4
X_A-M-X_B	175.7	176.2	176.4
τ[a]	-1.8	0.7	0.7
θ[b]	5.36	3.82	4.99
δ_P[c]	-0.182	-0.168	-0.154
H-C-P-C_{ring}[d]	-39.9, 174.8; -44.8, -53.3	-173.9, 40.1; 45.1, 53.1	46.4, 53.4; 41.3, -173.9

[a]The torsion angle C_A-X_A-X_B-C_B where C is the carbon atom bonded to phosphorus and X is the centroid. [b]The dihedral angle between the two C_5 rings. [c]Deviation of the P atom from the C_5 plane; a positive value means the P is closer to the Fe. [d]The torsion angle where H is the methyne hydrogen atom and the second C is the carbon atom of the C_5 ring bonded to the P atom.

Table 3 Ligands and metallocenes for comparison

	dippf	**dippf$^+$**	**dippc**	**dippc$^+$**
rel. E (gas phase, same M, kcal mol^{-1})	0.00	137.60	0.00	122.02
M-X	1.685, 1.690	1.755, 1.758	1.782, 1.793	1.682, 1.682
X_A-M-X_B	178.8	177.2	175.4	176.0
τ[a]	-144.1	-5.9	-82.1	-141.8
θ[b]	1.85	11.35	5.48	4.60
δ_P[c]	-0.056	-0.031	-0.073	-0.035
H-C-P-C_{ring}[d]	-44.1, 169.6; -39.9, -58.8	-39.7, 166.9; -40.2, -52.9	-44.1, 170.8; -40.4, -58.8	-43.1, 169.3; -42.3, -51.4

[a]The torsion angle C_A-X_A-X_B-C_B where C is the carbon atom bonded to phosphorus and X is the centroid. [b]The dihedral angle between the two C_5 rings. [c]Deviation of the P atom from the C_5 plane; a positive value means the P is closer to the Fe. [d]The torsion angle where H is the methyne hydrogen atom and the second C is the carbon atom of the C_5 ring bonded to the P atom.

	Fc	**Fc$^+$**	**Cc**	**Cc$^+$**
rel. E (gas phase, same M, kcal mol^{-1})	0.00	145.26	0.00	128.25
M-X	1.685, 1.685	1.748, 1.749	1.776, 1.779	1.678, 1.679
X_A-M-X_B	180.0	179.3	179.6	179.8
Cp ring torsion	0.0	-29.4	-0.6	-0.6

Table 4 Gaussian calculated (B3LYP/6-311+G**, SDD on Fe, Co, Re) ligands and metallocenes for comparison

	$[Re(CO)_3(dippf)Br]$ from Fe(III) XRD	**$[Re(CO)_3(dippf)Br]^+$ from XRD**	**$[Re(CO)_3(dippc)Br]$ from Fe(III) XRD**	**$[Re(CO)_3(dippc)Br]^+$ from XRD**
rel. E (gas phase, same M, kcal mol^{-1})	0.00	140.98	0.00	131.29
C-O (trans to P)	1.159, 1.159	1.155, 1.155	1.150, 1.150	1.145, 1.146
C-O (trans to Br)	1.170	1.166	1.162	1.157
Re-C (trans to P)	1.952, 1.957	1.957, 1.961	1.957, 1.951	1.967, 1.959
Re-C (trans to Br)	1.917	1.925	1.919	1.925
Re-Br	2.713	2.701	2.718	2.717
Re-P	2.603, 2.648	2.643, 2.610	2.675, 2.624	2.645, 2.590
M-X	1.679, 1.680	1.741, 1.741	1.764, 1.766	1.673, 1.673
Re-C-O (trans to P)	175.4, 177.6	175.4, 177.5	176.9, 175.0	175.8, 177.9
Re-C-O (trans to Br)	174.7	175.5	174.6	175.6
P-Re-P	94.3	97.7	95.9	95.6
Br-Re-P	89.8, 88.3	88.0, 89.8	87.8, 90.1	88.0, 90.1
X_A-M-X_B	175.7	177.7	176.7	176.8
τ^a	-1.5	-2.4	-2.8	1.4
θ^b	5.07	6.29	4.40	4.79
$\delta_P{}^c$	-0.176	-0.068	-0.200	-0.166
H-C-P-$C_{ring}{}^d$	174.2, -41.4; -45.1, -52.0	-53.6, -46.1; -41.4, 176.4	-44.0, -53.0; 174.3, -40.9	46.3, 52.6; -174.3, 41.7

[a]The torsion angle C_A-X_A-X_B-C_B where C is the carbon atom bonded to phosphorus and X is the centroid. [b]The dihedral angle between the two C_5 rings. [c]Deviation of the P atom from the C_5 plane; a positive value means the P is closer to the Fe. [d]The torsion angle where H is the methyne hydrogen atom and the second C is the carbon atom of the C_5 ring bonded to the P atom.

Table 5 Ligands and metallocenes for comparison

	dippf	**dippf$^+$**	**dippc**	**dippc$^+$**
rel. E (gas phase, same M, kcal mol^{-1})	0.00	135.76	0.00	122.21
M-X	1.692, 1.691	1.750, 1.752	1.781, 1.783	1.679, 1.678
X_A-M-X_B	178.8	177.5	178.7	178.7
τ^a	-143.9	-166.5	-142.6	-140.8
θ^b	2.20	1.45	2.97	1.71
$\delta_P{}^c$	-0.114	0.031	0.142	-0.034
H-C-P-$C_{ring}{}^d$	-45.5, -49.8; -42.9, 169.3	-41.1, -52.2; -41.1, 168.5	-44.9, -50.0; -43.4, 170.6	-42.8, -51.1; -42.1, 169.2

[a]The torsion angle C_A-X_A-X_B-C_B where C is the carbon atom bonded to phosphorus and X is the centroid. [b]The dihedral angle between the two C_5 rings. [c]Deviation of the P atom from the C_5 plane; a positive value means the P is closer to the Fe. [d]The torsion angle where H is the methyne hydrogen atom and the second C is the carbon atom of the C_5 ring bonded to the P atom.

	Fc	**Fc$^+$**	**Cc**	**Cc$^+$**
rel. E (gas phase, same M, kcal mol^{-1})	0.00	145.80	0.00	129.43
M-X	1.687, 1.687	1.748, 1.748	1.778, 1.778	1.674, 1.674
X_A-M-X_B	179.9	179.8	179.4	179.9
Cp ring torsion	0.0	-0.1	0.0	-8.9

Calculated estimates for energy required in one-electron oxidations of metallocene complexes

Table 6 Jaguar calculated (UB3LYP/6-311G*, LACV3P* on Re, Fe, Br, PBF/DCM solvation), *cf.* Roy *et al*.[11]

Complex	ΔE(g), kcal mol^{-1}	ΔG(g), kcal mol^{-1}	ΔE(soln), kcal mol^{-1}	ΔG(soln),[a] kcal mol^{-1}	E^{0}_{calc}, V
$[Re(CO)_3(dippf)Br]^{0/+}$	145.52	147.05	111.50	113.03	4.90
$[Re(CO)_3(dippc)Br]^{0/+}$	131.17	133.03	96.68	98.54	4.27
$dippf^{0/+}$	137.60	138.44	106.61	107.45	4.66
$dippc^{0/+}$	122.02	122.13	89.69	89.80	3.89
$[FeCp_2]^{0/+}$	145.26	150.58	124.58	129.89	5.63
$[CoCp_2]^{0/+}$	128.25	132.57	86.45	90.77	3.93

[a] ΔG(soln) = ΔG(g) + ΔE(soln) - ΔE(g)

Table 7 Gaussian calculated (UB3LYP/6-311+G**, SDD on Fe, Co, Re, DCM solvation), *cf.* Konezny *et al*.[12]

Complex	ΔE(g), kcal mol^{-1}	ΔG(g), kcal mol^{-1}	ΔE(soln), kcal mol^{-1}	ΔG(soln),[a] kcal mol^{-1}	E^{0}_{calc}, V
$[Re(CO)_3(dippf)Br]^{0/+}$	140.98	140.82	109.26	109.10	4.73
$[Re(CO)_3(dippc)Br]^{0/+}$	131.29	134.49	98.79	101.99	4.42
$dippf^{0/+}$	135.76	135.07	106.49	105.80	4.58
$dippc^{0/+}$	122.21	126.90	92.64	97.33	4.22
$[FeCp_2]^{0/+}$	145.80	145.59	108.14	107.93	4.68
$[CoCp_2]^{0/+}$	129.43	133.98	91.74	96.29	4.17

[a] ΔG(soln) = ΔG(g) + ΔE(soln) - ΔE(g)

These data show that while the gas-phase energies and free energies are reasonably consistent across both approaches, greater deviations emerge once solvation energies are included, with the ferrocene/ferrocenium couple in Jaguar particularly standing out. Since this couple would be used as the reference electrode, we have not calculated the potential with respect to this couple. The likely issues for such discrepancies and suggested pragmatic solutions have been reported previously,[11-12] and Adams *et al*. further suggested that explicit interaction with solvents and/or counterions might need to be considered as well,[13] further increasing conformational complexity.

Here, results indicate that problems seem to be linked, at least in part, to solvation corrections and we restrict ourselves to observing the general trends. These suggest that the cobaltocene couples are generally easier to oxidise than their ferrocene equivalents and that metallocene derivatisation appears to make oxidation easier compared to the unsubstituted metallocene, while the rhenium complexation of these ligands raises the energy difference again. It is noteworthy that the differences between complexes of the same metallocene are quite small, making them particularly susceptible to conformational and computational noise. We have commenced a computational study to further explore these issues and benchmark data at higher levels of theory and will report on these in due course.

References

1. K.-S. Gan and T. S. A. Hor, 1,1′-Bis(diphenylphosphino)ferrocene - Coordination Chemistry, Organic Synthesis and Catalysis. In *Ferrocenes: Homogeneous Catalysis, Organic Synthesis, Materials Science*; A. Togni and T. Hayashi, Eds.; VCH: Weinheim, Germany, 1995; pp 3-104.
2. A. Houlton, S. K. Ibrahim, J. R. Dilworth and J. Silver, *J. Chem. Soc., Dalton Trans.*, 1990, 2421.
3. B. Corain, B. Longato, G. Favero, D. Ajò. G. Pilloni, U. Russo and F. R. Kreissl, *Inorg. Chim. Acta*, 1989, **157**, 259.
4. B. Blass, R. H. Sánchez, V. A. Decker, M. J. Robinson, N. A. Piro, W. S. Kassel, P. L. Diaconescu and C. Nataro, *Manuscript submitted to Organometallics*.
5. a) Jaguar 8.5, Schrödinger-Inc., New York, NY, 2014; b) A. D. Bochevarov, E. Harder, T. F. Hughes, J. R. Greenwood, D. A. Braden, D. M. Philipp, D. Rinaldo, M. D. Halls, J. Zhang and R. A. Friesner, *Int. J. Quantum Chem.*, 2013, **113**, 2110-2142.
6. a) J. C. Slater, *Quantum Theory of Molecules and Solids, Vol. 4: The Self-Consistent Field for Molecules and Solids*, McGraw-Hill, New York, 1974; b) A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098-3100; c) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652; d) S. H. Vosko, L. Wilk and M. Nusair, *Can. J. Phys.*, 1980, **58**, 1200-1211; e) C. T. Lee, W. T. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785-789; f) B. Miehlich, A. Savin, H. Stoll and H. Preuss, *Chem. Phys. Lett.*, 1989, **157**, 200-206; g) P. J. Stephens, F. G. Devlin, C. F. Chabalowski and M. J. Frisch, *J. Phys. Chem.*, 1994, **98**, 11623.
7. D. J. Tannor, B. Marten, R. Murphy, R. A. Friesner, D. Sitkoff, A. Nicholls, B. Honig, M. Ringnalda and W. A. Goddard, *J. Am. Chem. Soc.*, 1994, **116**, 11875-11882.
8. Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. , lmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2013**.
9. a) D. Andrae, U. Häußermann, M. Dolg, H. Stoll and H. Preuß, *Theoret. Chim. Acta*, 1990, **77**, 123-141; b) M. Dolg, U. Wedig, H. Stoll and H. Preuss, *J. Chem. Phys.*, 1987, **86**, 866-872.
10. a) B. Marten, K. Kim, C. Cortis, R. A. Friesner, R. B. Murphy, M. N. Ringnalda, D. Sitkoff and B. Honig, *J. Phys. Chem.*, 1996, **100**, 11775; b) D. J. Tannor, B. Marten, R. B. Murphy, R. A. Friesner, D. Sitkoff, A. Nicholls, M. N. Ringnalda, W. A. Goddard III and B. Honig, *J. Am. Chem. Soc.*, 1994, **116**, 11875.
11. L. E. Roy, E. Jakubikova, M. G. Guthrie and E. R. Batista, *J. Phys. Chem. A*, 2009, **113**, 6745-6750.
12. S. J. Konezny, M. D. Doherty, O. R. Luca, R. H. Crabtree, G. L. Soloveichik and V. S. Batista, *J. Phys. Chem. C*, 2012, **116**, 6349-6356.
13. C. J. Adams, R. C. da Costa, R. Edge, D. H. Evans and M. F. Hood, *J. Org. Chem.*, 2010, **75**, 1168-1178.

XYZ coordinates for all calculated structures discussed

Jaguar calculated (UB3LYP/6-311G*, LACV3P* on Re, Fe, Br)

Table 8 [$Re(CO)_3$(dippf)Br], from XRD
E = -2098.97319235189 H

Re1	3.7346797571	8.0672589112	4.4797560230
Br2	4.3936559406	9.1181433632	2.0158946618
Fe3	3.7310042923	4.2588874738	1.9544953961
P4	1.7457219368	6.7379242155	3.3956359544
C5	2.1210173923	5.5472365984	2.0640064192
O6	2.9724821666	7.1101186408	7.2913544891
O7	5.7502289698	9.9663260891	5.8560629013
C8	2.9409546739	5.8618340837	0.9264152250
H9	3.4681471373	6.7926842171	0.7803818277
C10	2.9759434390	4.7253852325	0.0750370632
H11	3.5440404144	4.6404594343	-0.8398195822
O12	1.6973464105	10.3765410982	4.7585218167
C13	2.1909372545	3.6972304452	0.6702253130
H14	2.0564814309	2.6956500196	0.2883002776
C15	1.6562983829	4.1997478890	1.8887473319
H16	1.0347957579	3.6409459487	2.5707396960
C17	5.3258174593	4.7808003640	3.1955852836
C18	4.5609997870	3.7167404120	3.7780252012
H19	4.0612533104	3.7546715541	4.7328443620
C20	4.5743753155	2.6034644630	2.8930846400
H21	4.0630301942	1.6649987812	3.0495116413
C22	5.3322676923	2.9655248596	1.7444790449
H23	5.4894204786	2.3551540684	0.8671829129
C24	5.7873003594	4.3033872708	1.9210544440
H25	6.3436392779	4.8713582097	1.1931187490
P26	5.7163725745	6.3683548826	4.0399762360
H27	8.1059259886	5.1251463402	2.5107708340
H28	8.9753935514	6.5654898861	2.0005140718
H29	6.7155392261	5.7530060523	7.7230318641
C30	0.3907138220	7.8002899212	2.5732902066
H31	0.1119086496	8.5151409687	3.3530601565
C32	-0.8552245831	6.9967759748	2.1681939101
H33	-1.3911750988	6.5584523006	3.0102908692
H34	-1.5568331956	7.6632185081	1.6579040299
H35	-0.6054393921	6.1962982848	1.4670227024
C36	0.8865058803	8.6035993845	1.3645847065
H37	1.7560626939	9.2168178598	1.5853901959
H38	1.1435634128	7.9497325504	0.5277416945
H39	0.0817988780	9.2636977269	1.0260744438
C40	0.6815984165	5.7419245785	4.6033553795
H41	-0.0624039698	5.2537754765	3.9688009579
C42	-0.0673786153	6.6564027476	5.5871923355
H43	-0.6937675833	7.3980042769	5.0908460054

H44	-0.7254747085	6.0473518501	6.2140803638
H45	0.6124049921	7.1835605912	6.2561849910
C46	1.4263806460	4.6362121006	5.3611927096
H47	1.8859105900	3.9144971600	4.6885460529
H48	2.1969155407	5.0341375371	6.0200725462
H49	0.7154458827	4.0930354671	5.9919608463
C50	3.2694324802	7.4257727243	6.2147681721
C51	5.0469666606	9.2371969656	5.3107893945
C52	2.4372916028	9.5033918096	4.6486497286
H53	7.9766064590	8.4219192499	4.4547479933
H54	8.4124960576	8.7733335822	2.7895634055
H55	8.9415241501	6.1225858967	3.6974748363
H56	7.7495641417	4.1448064327	4.5416720924
H57	6.4995048524	3.6448517398	5.6712550186
H58	5.1372400882	5.4183222898	7.0232479232
C59	7.1097950760	7.0655070452	2.9544636147
H60	6.6265570512	7.2111296706	1.9848536403
C61	7.5899982876	8.4447230213	3.4319111373
H62	6.8105691214	9.1971950827	3.3634509759
C63	8.3381510718	6.1513890145	2.7879724541
C64	6.7299346240	5.8167239405	5.5693509962
H65	7.5797450382	6.5060451469	5.5350612533
C66	6.0325947150	6.0332657856	6.9150677623
H67	5.7481656124	7.0721154509	7.0773638822
C68	7.2826301757	4.3848900593	5.4955461389
H69	8.0368209036	4.2537631817	6.2778754769

Table 9 [$Re(CO)_3$(dippf)Br], from Fe(III) XRD

E = -2098.97450910502 H, G = -2098.480834 H, E(sl) = -2098.99105352488 H

Re1	7.7136647262	2.6716547822	2.6769013028
Br2	5.6916946293	4.2211498314	3.7430513415
P3	9.3969463445	4.6330746169	3.0466919101
Fe4	8.9866540556	4.7889569487	6.5567468382
P5	8.0557009057	1.6307982534	5.0805286868
O6	9.7208336435	0.9351757644	1.1440714161
C7	11.5380506619	3.9829828101	1.2647064274
H8	12.6083455775	3.7822517715	1.1570644489
H9	11.3087579779	4.8425028416	0.6347758796
H10	11.0093131106	3.1193440669	0.8622912049
C11	11.7044993918	3.0373443291	3.5912136968
H12	12.7922983179	2.9500202435	3.5074326064
H13	11.2769265106	2.0990480522	3.2395199901
H14	11.4627646136	3.1451342021	4.6489010657
C15	9.5364530869	-0.2541790215	6.7187332181
H16	10.5403574075	-0.6316408011	6.9377501018
H17	8.8764773876	-1.1218040230	6.6756259604
H18	9.2281515834	0.3582614343	7.5649738643
C19	8.9939573811	1.5862586057	1.7750220595
C20	11.2161371618	4.2212975245	2.7481059010
H21	11.7579337213	5.1135995394	3.0732698592
C22	9.1615453409	6.0976145849	1.8601847215
H23	9.2467005601	5.6324188391	0.8732875310
C24	7.2814796149	3.4955392028	0.9706865826
O25	7.0110650374	3.9469399321	-0.0512387517
C26	6.3257447969	1.3619272870	2.2958835959
O27	5.4946102307	0.6263476508	1.9947804151
C28	9.4592044304	5.4896307673	4.6669862204
C29	7.2989790610	3.7021911780	7.0154635161
H30	6.3503350334	3.9219008663	6.5549708355
C31	8.2970113402	2.8172806292	6.4821474759
C32	9.5656757514	0.5081182816	5.3802364329
H33	10.3827761579	1.2324894222	5.4253948055
C34	9.9068139740	-0.4586955934	4.2374701565
H35	10.1447278017	0.0498819089	3.3086572820
H36	9.1062105966	-1.1676686066	4.0258821338
H37	10.7878391471	-1.0443461122	4.5196556979
C38	6.6296863498	0.5639625285	5.7659875249
H39	6.9339249577	0.3794825585	6.8009337752
C40	5.2605267028	1.2553264701	5.7998246977
H41	4.5337692270	0.5616331666	6.2353188403
H42	4.9056374767	1.5315170568	4.8081407190
H43	5.2536900592	2.1532003806	6.4123223178
C44	6.4962154644	-0.7924913074	5.0553813001
H45	5.6804599327	-1.3533662173	5.5212545068
H46	7.3889310904	-1.4097708988	5.1305291827
H47	6.2434392424	-0.6872256585	4.0007390807

C48	9.4465818085	2.9332490843	7.3438796713
H49	10.3913568701	2.4271985137	7.2279266884
C50	9.1412314456	3.8441585406	8.3934338376
H51	9.8172253005	4.1532228727	9.1775455050
C52	7.8137962456	4.3149439487	8.1917560306
H53	7.3031736546	5.0553710621	8.7902026732
C54	10.5853008477	5.6542113555	5.5466886792
H55	11.5652714820	5.2206021405	5.4267430804
C56	10.1912484174	6.4853332601	6.6310479403
H57	10.8094437936	6.7576230901	7.4743380949
C58	8.8298091860	6.8509408712	6.4347133121
H59	8.2276616431	7.4442733063	7.1074467731
C60	8.3718251658	6.2378261207	5.2362645610
H61	7.3655295952	6.2649566998	4.8511287765
C62	7.7754612225	6.7541861832	1.9432681798
H63	7.6381227396	7.4031494645	1.0730431458
H64	7.6920593806	7.3836233369	2.8308268186
H65	6.9529465480	6.0432993109	1.9651640590
C66	10.2443675263	7.1785745707	1.9986301562
H67	10.0368535235	7.9883626573	1.2924815402
H68	11.2529274404	6.8215045031	1.7885590459
H69	10.2415334241	7.6148292318	3.0002860032

Table 10 $[Re(CO)_3(dippf)Br]^+$, from XRD

E = -2098.74260904001 H, G = -2098.246498 H, E(sl) = -2098.81336546232 H

Re1	7.7139066972	2.6782216541	2.7194532035
Br2	5.7712048328	4.2461072353	3.8745475350
P3	9.4293020757	4.6182680171	2.9877099530
Fe4	8.9689266091	4.7747421365	6.5606378246
P5	8.0477780528	1.5392796853	5.0739075124
O6	9.6675874219	0.9170574109	1.1416785347
C7	11.5478625281	3.9187857944	1.2205279244
H8	12.6154308976	3.7121169492	1.1074191072
H9	11.3159539916	4.7600560997	0.5679034365
H10	11.0132902878	3.0448140703	0.8492141613
C11	11.7355834567	3.0319208181	3.5692710219
H12	12.8185821998	2.9257358417	3.4632251138
H13	11.2871817111	2.0907226296	3.2534564160
H14	11.5248910816	3.1648785506	4.6326379448
C15	9.5350851092	-0.3386897109	6.7084193666
H16	10.5368286272	-0.7183372266	6.9285168002
H17	8.8783619236	-1.2067935595	6.6435702611
H18	9.2157428894	0.2492006590	7.5700297338
C19	8.9617689214	1.5735010546	1.7810745047
C20	11.2478295157	4.2002987059	2.7030619178
H21	11.7988901051	5.0997887938	2.9936797906
C22	9.1739779243	6.0819384193	1.8018451079
H23	9.2298530910	5.5921287568	0.8246238338
C24	7.2460417285	3.5047218178	1.0184468352
O25	6.9483256960	3.9523496036	0.0073460967
C26	6.2932651470	1.3970317256	2.3330147607
O27	5.4449844174	0.6907414365	2.0278829957
C28	9.4994897775	5.5307539505	4.5988657459
C29	7.2589116090	3.6080422056	7.0217868214
H30	6.3130055425	3.8146895649	6.5470151501
C31	8.2489272376	2.7045630209	6.5212560616
C32	9.5736699605	0.4452480242	5.3831100029
H33	10.3836992500	1.1793790543	5.4375844261
C34	9.9314036304	-0.5019245014	4.2275660777
H35	10.1563289997	0.0199399315	3.3031368351
H36	9.1477799912	-1.2279901096	4.0135230104
H37	10.8252072050	-1.0685526594	4.5030334818
C38	6.6179850019	0.4669986518	5.7429554745
H39	6.9192852022	0.2528942085	6.7731654086
C40	5.2485309223	1.1559083434	5.7831592163
H41	4.5190462016	0.4425951097	6.1767618592
H42	4.9047081162	1.4722383288	4.7999653355
H43	5.2220929212	2.0243095808	6.4386650718
C44	6.5075911313	-0.8706832433	4.9925001084
H45	5.6995355528	-1.4525677577	5.4434201006
H46	7.4076626712	-1.4784107980	5.0554454949
H47	6.2542197413	-0.7419059128	3.9410368427

C48	9.3941173545	2.8541072414	7.3704516027
H49	10.3405735278	2.3492219868	7.2615217235
C50	9.0985491817	3.7971313471	8.3960708152
H51	9.7690540288	4.1058424875	9.1849483022
C52	7.7691755964	4.2643760608	8.1799029574
H53	7.2433974711	4.9999377127	8.7712861829
C54	10.6000577311	5.6750370107	5.5007273730
H55	11.5785275554	5.2341285896	5.3903688546
C56	10.1927311127	6.4782954592	6.6025808008
H57	10.8076597689	6.7527282685	7.4475340105
C58	8.8303113145	6.8461737241	6.3912184784
H59	8.2206178589	7.4487531672	7.0488191762
C60	8.4037690408	6.2569847906	5.1671033217
H61	7.4022607197	6.2800573377	4.7661850923
C62	7.7970851043	6.7543569952	1.9076870884
H63	7.6383844638	7.3672407579	1.0167766690
H64	7.7488814667	7.4291223045	2.7654658740
H65	6.9658077704	6.0569335441	1.9823247360
C66	10.2775128797	7.1469296638	1.8888660343
H67	10.0720552044	7.9307699586	1.1550416514
H68	11.2772131840	6.7683160471	1.6773346694
H69	10.2956034978	7.6296945095	2.8698962965

Table 11 [$Re(CO)_3$(dippc)Br], from Fe(III) XRD

E = -2120.59874648084 H, G = -2120.106727 H, E(sl) = -2120.61562435694 H

Re1	7.6987332612	2.6925713419	2.7047553897
Br2	5.7053173451	4.2572655630	3.8008922760
P3	9.4011312960	4.6580207333	3.0379544856
Co4	8.9755346055	4.8057643872	6.5777072168
P5	8.0417347971	1.6016853319	5.0999473179
O6	9.6601984120	0.9388388419	1.1343880399
C7	11.5320495611	3.9632284521	1.2557036923
H8	12.6021580788	3.7597564690	1.1481396263
H9	11.3016707670	4.8126600864	0.6121290060
H10	11.0017506689	3.0936184552	0.8684451915
C11	11.6916409617	3.0451971875	3.5922941519
H12	12.7786733030	2.9446204507	3.5099857763
H13	11.2535175189	2.1083504283	3.2487808898
H14	11.4496886065	3.1633740252	4.6492211494
C15	9.5326184872	-0.2900395152	6.7144355008
H16	10.5362318054	-0.6706695686	6.9301022167
H17	8.8723225631	-1.1570111198	6.6574666029
H18	9.2213625265	0.3114769946	7.5682982260
C19	8.9549983396	1.5976777075	1.7812257564
C20	11.2154651821	4.2258237815	2.7364236478
H21	11.7676081902	5.1175453754	3.0470807215
C22	9.1525264965	6.0885133400	1.8159073930
H23	9.1931853587	5.5960615581	0.8390472275
C24	7.2541904082	3.5166958945	1.0038241588
O25	6.9694754941	3.9565462194	-0.0194571759
C26	6.2977766895	1.4013320680	2.3187144988
O27	5.4579370441	0.6824009433	2.0017061061
C28	9.4826950181	5.5628778031	4.6237802020
C29	7.2779238152	3.6732713920	7.0288806942
H30	6.3348788764	3.8973952659	6.5568700511
C31	8.2536999799	2.7438303907	6.5288690133
C32	9.5632129686	0.4917782544	5.3877091670
H33	10.3725902757	1.2243767249	5.4514413602
C34	9.9218700668	-0.4555056650	4.2337843571
H35	10.1629481725	0.0672675493	3.3140851806
H36	9.1288182686	-1.1678897201	4.0053029312
H37	10.8052850040	-1.0381273385	4.5146714732
C38	6.6195483109	0.5021830480	5.7397109728
H39	6.9215502791	0.2855612426	6.7691689109
C40	5.2526248747	1.1958300193	5.7958491750
H41	4.5216505924	0.4918643458	6.2073431300
H42	4.8992113336	1.5080304257	4.8142067870
H43	5.2516245855	2.0730022287	6.4393635244
C44	6.4910311892	-0.8324077568	4.9882406789
H45	5.6765861588	-1.4102706382	5.4361038339
H46	7.3862265480	-1.4488557101	5.0464726499
H47	6.2399381810	-0.6977307505	3.9369187118

C48	9.3872764402	2.8858653395	7.3852648880
H49	10.3345791412	2.3778197169	7.2911839268
C50	9.0584023019	3.7783479352	8.4639637144
H51	9.7223791594	4.0554133379	9.2702868640
C52	7.7464248455	4.2375887263	8.2589152905
H53	7.2141507308	4.9590451438	8.8615742050
C54	10.5856390348	5.7135767159	5.5160468117
H55	11.5692891709	5.2845098222	5.4029873443
C56	10.2082316593	6.5991198287	6.5828287831
H57	10.8468371504	6.8990046386	7.4014629481
C58	8.8676508666	6.9672975117	6.3869296647
H59	8.2687824520	7.5877992528	7.0377957597
C60	8.3905667013	6.2761259955	5.2264342785
H61	7.3811980809	6.3019790156	4.8466404214
C62	7.7831283007	6.7737755482	1.9406662721
H63	7.6222580096	7.4084749758	1.0638534902
H64	7.7475386890	7.4217338876	2.8192511453
H65	6.9482358146	6.0797906920	2.0103063451
C66	10.2602112206	7.1501802155	1.8877403544
H67	10.0470424854	7.9436261307	1.1645577966
H68	11.2541301247	6.7645467013	1.6573077549
H69	10.2985579515	7.6142860506	2.8764945330

Table 12 [$Re(CO)_3$(dippc)Br], from Co(III) XRD

E = -2120.59855901897 H

Re1	10.8518482804	15.6980859789	11.9501007712
Br2	12.5913025278	13.9412656210	13.1775486387
Co3	12.6595438092	17.3387244962	15.8242301359
P4	12.6031395321	17.6219602420	12.2706991674
C5	13.4272512029	17.8798849546	13.8819943233
P6	9.6394848877	16.0065080485	14.2925934386
C7	14.2586558289	16.9192884206	14.5566824200
H8	14.4410000000	15.9111801866	14.2194745780
C9	14.8250253776	17.5284884921	15.7216181849
H10	15.4921541380	17.0462369011	16.4211454881
C11	14.2582523182	18.8062070845	15.8524586875
H12	14.4277073868	19.5075114223	16.6571565869
C13	13.3831521442	19.0220564078	14.7328184927
H14	12.8239917389	19.9297417438	14.5662831274
C15	10.6953702175	16.3931858178	15.7512630014
C16	10.6869689350	17.5663962398	16.5643198804
H17	10.0868941780	18.4508911522	16.4155237679
C18	11.5767062759	17.3761561270	17.6789657605
H19	11.7575907068	18.0965033795	18.4640841869
C20	12.1759936882	16.1131545463	17.5429902276
H21	12.9310465874	15.6857880760	18.1865751255
C22	11.7062070290	15.5422692173	16.3173368509
H23	12.0456668904	14.6127569931	15.8900753075
C24	11.9812091213	19.3607108637	11.8687670888
H25	12.7921365302	20.0244176326	12.1821446523
C26	11.7410030741	19.5785313375	10.3669499351
H27	10.9557994125	18.9315404146	9.9766439799
H28	12.6352903187	19.4238191819	9.7632003894
H29	11.4167420276	20.6105756512	10.2009308516
C30	10.7233544106	19.7385672800	12.6603199015
H31	10.5066298763	20.8027953951	12.5229498815
H32	10.8248908485	19.5587584462	13.7310020665
H33	9.8543911636	19.1841700910	12.3075663174
C34	14.0963068012	17.4874365107	11.1056919832
H35	13.6388723648	17.4446475467	10.1124349400
C36	14.9159525548	16.2022342606	11.2966891089
H37	15.5926606190	16.0815701991	10.4452050986
H38	14.3115581992	15.3012981804	11.3743981356
H39	15.5356277178	16.2622352330	12.1935403309
C40	15.0354748296	18.7004258331	11.1738901922
H41	15.8736957585	18.5477449543	10.4869494667
H42	15.4556055973	18.8178299201	12.1756091640
H43	14.5613526049	19.6419593150	10.8952946700
C44	8.3602694731	17.4038153878	14.4794619488
H45	8.9975144224	18.2906133141	14.5401227799
C46	7.5277769864	17.3312077534	15.7730534435
H47	7.0339915338	18.2944223071	15.9376018777

H48	8.1183942577	17.1117402610	16.6618428250
H49	6.7382749056	16.5810382266	15.7032837046
C50	7.4321642299	17.6151199871	13.2747525596
H51	6.7479637016	18.4411300633	13.4941402556
H52	6.8176422175	16.7427152980	13.0515645595
H53	7.9659540980	17.8757040318	12.3665628799
C54	8.6779697460	14.4938778954	14.9435276140
H55	8.3838104665	14.8039480561	15.9512040638
C56	7.4017249997	14.1911095656	14.1436587502
H57	6.9023290479	13.3264404844	14.5918071323
H58	7.6086617287	13.9311337493	13.1060388093
H59	6.6842257452	15.0098577219	14.1504254477
C60	9.5182364467	13.2179098904	15.0781430612
H61	8.8819622293	12.4222169731	15.4793461876
H62	10.3543648109	13.3356162185	15.7637887081
H63	9.9201304446	12.8744921862	14.1259617688
O64	8.9496163327	17.3959963140	10.2486778701
C65	9.6573822260	16.7892641173	10.9424710440
O66	9.1350670374	13.2141661805	11.2806192230
C67	9.7417073225	14.1436867050	11.5832328309
C68	11.7839224609	15.2860865312	10.2969738837
O69	12.2928868189	15.0167145913	9.3016393111

Table 13 $[Re(CO)_3(dippc)Br]^+$, from XRD

E = -2120.38970926619 H, G = -2119.894725 H, E(sl) = -2120.46156126064 H

Re1	10.8642225224	15.7051987203	11.9356284062
Br2	12.6085197497	13.9905640412	13.2053763778
Co3	12.6652988487	17.3284171465	15.8034521795
P4	12.5707158905	17.6257980198	12.2420235509
C5	13.3590966340	17.8488574613	13.9053792343
P6	9.6550838562	16.0252098588	14.2414479124
C7	14.2243810970	16.8920380282	14.5381448940
H8	14.3972453514	15.8866446431	14.1864072899
C9	14.7226152398	17.4564179362	15.7463602322
H10	15.3741741358	16.9622569235	16.4524456230
C11	14.1596575379	18.7571162384	15.8910290209
H12	14.3109357692	19.4292793386	16.7233056304
C13	13.3243354944	18.9985411146	14.7648836035
H14	12.7536517722	19.8997219229	14.6067533637
C15	10.7677652367	16.4236892021	15.6904025695
C16	10.7521795385	17.5952362256	16.5258094056
H17	10.1597851288	18.4829884019	16.3732628581
C18	11.6661736598	17.4120637455	17.6025221793
H19	11.8818377964	18.1316067755	18.3790400173
C20	12.2795086996	16.1377867060	17.4387535626
H21	13.0512362456	15.7157507110	18.0660299115
C22	11.7466302075	15.5416933226	16.2602180741
H23	12.0782493242	14.6171546854	15.8149314198
C24	11.9778563094	19.3789166073	11.8644140141
H25	12.7901479839	20.0341323111	12.1932987226
C26	11.7712224439	19.5980712332	10.3558599617
H27	10.9914580318	18.9545451544	9.9484601364
H28	12.6776597532	19.4441508795	9.7709807487
H29	11.4539548855	20.6306393633	10.1869208142
C30	10.7051114593	19.7665501490	12.6269780644
H31	10.4949389431	20.8279956912	12.4699196379
H32	10.7801927450	19.6073586769	13.7046441116
H33	9.8408810387	19.2109058256	12.2656334694
C34	14.1284462248	17.5154642735	11.1579689032
H35	13.6963093726	17.4964590023	10.1523466679
C36	14.9450955592	16.2268698796	11.3350143605
H37	15.6273320124	16.1270987934	10.4869666927
H38	14.3431043982	15.3227933432	11.3849448670
H39	15.5661885554	16.2676308177	12.2329632991
C40	15.0554102626	18.7344902118	11.2795021797
H41	15.9019669645	18.6053309920	10.5998414799
H42	15.4712781472	18.8276154026	12.2868254800
H43	14.5814192303	19.6805210498	11.0190098121
C44	8.3995963257	17.4372935025	14.4680139568
H45	9.0434297793	18.3215713693	14.5011689932
C46	7.5984894107	17.3711999616	15.7811559744
H47	7.1084877954	18.3343056579	15.9501154386

H48	8.2009970187	17.1557113045	16.6647865685
H49	6.8082031945	16.6214748949	15.7347513418
C50	7.4435873272	17.6447528371	13.2838787747
H51	6.7909128769	18.4941927842	13.5040565905
H52	6.7978048763	16.7860294293	13.1030327538
H53	7.9574302545	17.8688289932	12.3548320911
C54	8.7306878092	14.5262958634	14.9768074736
H55	8.4538487029	14.8629625494	15.9808259196
C56	7.4364503568	14.2220317055	14.2029477062
H57	6.9232499020	13.3963247051	14.7023945169
H58	7.6284586902	13.9011355794	13.1797552801
H59	6.7382453611	15.0564027424	14.1733477821
C60	9.5631579115	13.2459625383	15.1196873814
H61	8.9186710323	12.4628898189	15.5289131888
H62	10.4010591906	13.3516808817	15.8071511827
H63	9.9571208357	12.8880649391	14.1699646057
O64	8.9615870675	17.3902898740	10.2206143736
C65	9.6658289220	16.7850292086	10.9105005704
O66	9.1519570959	13.2076069524	11.2894852876
C67	9.7566502569	14.1384886803	11.5723245610
C68	11.8078929043	15.2742062201	10.2851658119
O69	12.3360011090	15.0000279361	9.3064717383

Table 14 dippf

E = -1666.42021394186 H, G = -1665.951991 H, E(sl) = -1666.42954449704 H

P1	11.5938152541	6.7629461895	7.7019766422
Fe2	8.8326983276	4.8144091602	6.5078707924
P3	7.6139983821	1.7884630999	5.2890792703
C4	11.6691170723	9.1220954238	9.2471800784
H5	11.1246902740	9.9210431312	9.7610197448
H6	12.4281957098	9.5980841568	8.6233949345
H7	12.1854448697	8.5346289426	10.0133634576
C8	9.5402253504	7.7875873061	9.3372556206
H9	9.0159324372	8.6499899062	9.7630013020
H10	9.9114763989	7.1840940355	10.1713712340
H11	8.8108868774	7.1889133941	8.7918915680
C12	9.6466539836	-0.0757990328	6.3074979500
H13	10.7072323632	-0.3483675895	6.2699145223
H14	9.0768429608	-0.9945690147	6.1467883435
H15	9.4326853178	0.2679579207	7.3211986334
C16	10.6938500282	8.2538526563	8.4385305839
H17	10.2802885898	8.8623562105	7.6270902495
C18	12.9167559779	7.6064729688	6.6280495433
H19	13.5318100414	8.1309830887	7.3688154994
C20	10.4262422187	6.1821212095	6.3995571766
C21	6.9241615667	4.1045292279	6.8463234333
H22	6.0817778448	4.3361400252	6.2103719552
C23	7.8188579591	2.9954176583	6.6641278731
C24	9.3352922319	0.9827544138	5.2407730446
H25	9.9984129005	1.8383172477	5.4081759368
C26	9.6330843897	0.4461890995	3.8310782803
H27	9.4888058136	1.2145692334	3.0678462686
H28	8.9876755760	-0.3969642590	3.5692041816
H29	10.6687713805	0.0957189977	3.7637433903
C30	6.5098437611	0.4766945368	6.1007989142
H31	7.0185587339	0.0770701130	6.9840391660
C32	5.1819543072	1.0999036395	6.5511305600
H33	4.5254833101	0.3280054928	6.9669172482
H34	4.6522299134	1.5618176002	5.7113982387
H35	5.3235914077	1.8617724186	7.3194188896
C36	6.2472576690	-0.6665334874	5.1096368361
H37	5.5813662401	-1.4128880767	5.5558387665
H38	7.1600458903	-1.1854272110	4.8095526042
H39	5.7641253352	-0.2961227020	4.2000287968
C40	8.8204483278	3.1079549478	7.6886886733
H41	9.6746929317	2.4621192046	7.8213962690
C42	8.5321009590	4.2500784084	8.4878079165
H43	9.1302829408	4.6077992581	9.3129712658
C44	7.3553828507	4.8644544964	7.9697521157
H45	6.8866796620	5.7636111840	8.3425808736
C46	9.2219056686	6.7663709645	5.8840465119
H47	8.7256718037	7.6427559409	6.2739079231

C48	8.7578317620	5.9794125845	4.7910939986
H49	7.8552876582	6.1502054356	4.2218457311
C50	9.6680467116	4.8997293317	4.6106413935
H51	9.5747318645	4.1118856043	3.8774319455
C52	10.6815146395	5.0114480663	5.6049281409
H53	11.5020865061	4.3241191429	5.7516333688
C54	13.8142886729	6.5511305303	5.9662630845
H55	14.6750912884	7.0298591763	5.4876737787
H56	13.2788835622	5.9990122039	5.1895404787
H57	14.1956682134	5.8283807517	6.6925700909
C58	12.4086833439	8.6224149812	5.6005803025
H59	13.2492254179	9.0817290760	5.0680621125
H60	11.8359407575	9.4319451044	6.0596386607
H61	11.7688278122	8.1449846809	4.8541925434

Table 15 dippf^{+}

E = -1666.20093730061 H, G = -1665.73137 H, E(sl) = -1666.25965707865 H

P1	9.2222766259	4.7119965133	2.8793099384
Fe2	9.0781714412	4.7207316571	6.5453159024
P3	8.6184304815	1.3166440775	5.2370295037
C4	11.2246377271	4.2822359979	0.9479156341
H5	12.2674187616	4.0361031682	0.7305225366
H6	10.9729045302	5.1632378808	0.3570291597
H7	10.6146955725	3.4482518152	0.5901966055
C8	11.6365503830	3.3207076881	3.2340776528
H9	12.7061122223	3.2262699750	3.0263544818
H10	11.1547597628	2.3870947853	2.9403234202
H11	11.5187622166	3.4168523003	4.3148530723
C12	8.5842260909	-0.7089373629	7.3426875650
H13	9.1578552631	-1.4899918428	7.8521402738
H14	7.6384714954	-1.1585304314	7.0341239675
H15	8.3610775332	0.0655855522	8.0811332187
C16	11.0499330780	4.5088532985	2.4566033217
H17	11.5869404212	5.4219005039	2.7323263950
C18	8.6549303437	6.1246830556	1.7433238919
H19	8.8379200745	5.6849799405	0.7565034425
C20	9.2999898956	5.6000167825	4.4944829540
C21	7.6734823313	3.2704926670	7.2732467172
H22	6.6239979225	3.2479863882	7.0228299777
C23	8.7026387963	2.5115669927	6.6377440124
C24	9.3838962179	-0.1669938068	6.1525048145
H25	10.3149585339	0.2630617707	6.5397897444
C26	9.7901145037	-1.2688617457	5.1607284023
H27	10.3924118909	-0.8726621640	4.3396856340
H28	8.9288019681	-1.7780589809	4.7263206670
H29	10.3880922495	-2.0274929003	5.6750259611
C30	6.7604220794	1.0089953977	5.1105967419
H31	6.3406234965	0.9393159023	6.1195345831
C32	6.1009057055	2.1773203573	4.3587577902
H33	5.0168961843	2.0350194608	4.3249939585
H34	6.4636031739	2.2316688665	3.3305463955
H35	6.2894487400	3.1503044037	4.8159018897
C36	6.4683868455	-0.3031223332	4.3677647439
H37	5.3914437018	-0.3979431952	4.2039431051
H38	6.7876575806	-1.1848198463	4.9224489297
H39	6.9490447960	-0.3271278209	3.3860106826
C40	9.9331587485	2.9139976347	7.2598657443
H41	10.9181647801	2.5623741164	6.9876835810
C42	9.6496362030	3.8176357240	8.3251797177
H43	10.3720999076	4.2550343652	8.9991139032
C44	8.2430276298	4.0481969385	8.3259189398
H45	7.6992901297	4.6959080684	8.9985597817
C46	10.4172651185	5.8909708696	5.3345376923
H47	11.4458584429	5.6375208673	5.1275473420

C48	9.9686299632	6.6042053506	6.4860187327
H49	10.5982451225	6.9827248321	7.2784029939
C50	8.5517422682	6.7267629048	6.3956581821
H51	7.9042543761	7.2127337279	7.1110740932
C52	8.1414611389	6.0695950937	5.1994681302
H53	7.1195655686	5.9555506373	4.8701953063
C54	7.1417109584	6.3564441461	1.8499673718
H55	6.8074563141	7.0077947968	1.0372887732
H56	6.8666489881	6.8547695609	2.7827790995
H57	6.5770203408	5.4245524651	1.7779259431
C58	9.4401576199	7.4349873809	1.8526377963
H59	9.1130955222	8.1357077514	1.0776788376
H60	10.5152320498	7.2937450596	1.7269056645
H61	9.2764235164	7.9224239678	2.8179662353

Table 16 dippc

E = -1688.04303299679 H, G = -1687.573532 H, E(sl) = -1688.05162160894 H

P1	12.3393554280	4.7873582872	5.4508211323
Co2	8.8122302824	4.8729148797	6.3508054485
P3	7.6482023624	1.6420060877	5.4707754290
C4	14.6093787972	5.4573562880	6.9827388467
H5	15.0239930120	5.8382491619	7.9216516032
H6	15.0931408467	6.0041190590	6.1709177062
H7	14.9027551907	4.4057735303	6.8998241892
C8	12.4832523014	4.9982958984	8.2498197655
H9	12.9022064176	5.4783688011	9.1407093281
H10	12.7109827854	3.9297310208	8.3126686125
H11	11.3993468384	5.1091871599	8.2883575623
C12	9.9619848696	0.0191466974	6.2773655488
H13	11.0279811531	-0.1630927284	6.1026765985
H14	9.4615389573	-0.9521187593	6.2397381440
H15	9.8581772895	0.4003202197	7.2951154426
C16	13.0811161301	5.6147754923	6.9780990395
H17	12.8431522922	6.6838430946	6.9633994096
C18	13.1978306927	5.7347692771	4.0449168171
H19	14.2504705073	5.4551771261	4.1709939086
C20	10.6491069207	5.5157590582	5.3639401062
C21	6.9926439685	4.0226043705	6.9547463737
H22	6.0759621389	4.1630725703	6.3983372554
C23	7.9133867724	2.9247546970	6.7580254298
C24	9.4140190653	0.9867095152	5.2194950355
H25	10.0146568703	1.9020705658	5.2543633690
C26	9.5657410124	0.3980761320	3.8075412617
H27	9.2466763235	1.1067397368	3.0397036631
H28	8.9736169218	-0.5125152804	3.6771673992
H29	10.6114767675	0.1379535653	3.6113386366
C30	6.7828804058	0.2829505214	6.4701279159
H31	7.4377422153	-0.0250409197	7.2917318520
C32	5.4759549455	0.8168626229	7.0703197576
H33	4.9526242590	0.0180755093	7.6067207678
H34	4.7998372244	1.1854091973	6.2917152176
H35	5.6501165173	1.6306407671	7.7767550170
C36	6.4993983369	-0.9278702363	5.5695261555
H37	5.9712734443	-1.7062246023	6.1306841423
H38	7.4096426667	-1.3787397102	5.1683258972
H39	5.8681658217	-0.6480772657	4.7203080856
C40	8.9891812536	3.1627482902	7.6490820091
H41	9.8931943678	2.5789035107	7.7339798184
C42	8.6959938503	4.3353044289	8.4334638050
H43	9.3304691946	4.7492650903	9.2042914019
C44	7.4321906155	4.8240965434	8.0486853522
H45	6.9409719035	5.7074068683	8.4303716875
C46	10.0613924749	6.6470462158	6.0588086711
H47	10.5245355052	7.1991135967	6.8637876822

C48	8.7871141311	6.8943508069	5.5259620164
H49	8.0887181328	7.6479000143	5.8613132358
C50	8.5326077030	5.8910225021	4.5322790270
H51	7.6285384265	5.7937362150	3.9475580162
C52	9.7039478601	5.0956853474	4.3874539262
H53	9.8206270060	4.2634090499	3.7091041732
C54	12.7440234322	5.1868015075	2.6848304529
H55	13.3484969321	5.6189133749	1.8804405525
H56	11.7007885671	5.4403899686	2.4786726080
H57	12.8441456860	4.0994782176	2.6303974199
C58	13.0821205317	7.2612628909	4.0931977134
H59	13.6447252983	7.7143024405	3.2690829916
H60	13.4744317430	7.6821297755	5.0223315631
H61	12.0418803941	7.5823093149	3.9960367586

Table 17 dippc^{+}

E = -1687.84857819475 H, G = -1687.3789 H, E(sl) = -1687.90869850681 H

P1	9.0580409616	4.7078887101	2.9823938667
Co2	9.1511119490	4.7576500063	6.5437346740
P3	7.0168319036	4.7425844541	9.3932319062
C4	10.9710699870	4.0667667641	1.0335799788
H5	11.9959352403	3.7729560564	0.7912977674
H6	10.7221866994	4.9198145116	0.4003386488
H7	10.3198343731	3.2342689785	0.7504651803
C8	11.4149623111	3.2173777861	3.3614125034
H9	12.4618288378	3.0336747706	3.1033239111
H10	10.8622651989	2.2957993438	3.1584451242
H11	11.3727260621	3.4036555741	4.4369478523
C12	6.9372166612	2.1494892566	10.7269213722
H13	6.3688445366	1.2252375633	10.8673601137
H14	7.1734523758	2.5320473094	11.7222383005
H15	7.8779658599	1.8810558211	10.2392454432
C16	10.8615517079	4.3873607544	2.5328825145
H17	11.4559551264	5.2840442214	2.7386458011
C18	8.5858429904	6.1610778670	1.8569116924
H19	8.6827986385	5.7076827063	0.8638672036
C20	9.2077320273	5.5975324618	4.6006626213
C21	9.6969376971	3.8812145645	8.3466873626
H22	10.3189451109	4.3467979445	9.0957541620
C23	8.2651224390	3.9426832983	8.2816128162
C24	6.1167508948	3.1484058833	9.9029172436
H25	5.9031990996	2.6885386856	8.9305944337
C26	4.7573516247	3.4679471148	10.5447963000
H27	4.1654802424	4.1461742612	9.9260831298
H28	4.8569211280	3.9199826464	11.5329026283
H29	4.1832634261	2.5454437996	10.6689654265
C30	8.0881464687	5.2586953541	10.8595156208
H31	8.7864420228	4.4493220423	11.0983224194
C32	8.8807610796	6.5268431775	10.5003397066
H33	9.5235673696	6.8164776762	11.3364541453
H34	8.2077925844	7.3653726320	10.3012828170
H35	9.5231512098	6.4027464866	9.6257534560
C36	7.2182764483	5.5353944561	12.0959478630
H37	7.8384178757	5.9481640568	12.8963939469
H38	6.7432438932	4.6368838557	12.4887473761
H39	6.4342556273	6.2676786044	11.8825541374
C40	7.8943227093	3.2228829727	7.0902902962
H41	6.8889596840	3.1147673606	6.7094023299
C42	9.0637471900	2.6978982609	6.4722442970
H43	9.0939881849	2.1273615485	5.5558939656
C44	10.1832237397	3.1117705492	7.2482021882
H45	11.2212664948	2.9005571323	7.0356257390
C46	10.3572245318	5.9851945914	5.3643641518
H47	11.3858285916	5.7821226465	5.1066626600

C48	9.9284681910	6.6690259165	6.5392250997
H49	10.5722697640	7.0633998852	7.3121545175
C50	8.5042090395	6.7068230304	6.5302942118
H51	7.8679762041	7.1119843105	7.3031952889
C52	8.0627620158	6.0350343484	5.3556432229
H53	7.0320801727	5.8520945225	5.0910332181
C54	7.1080384176	6.5374431758	2.0340231453
H55	6.8016630190	7.2235863374	1.2398086026
H56	6.9282179031	7.0540880806	2.9807794882
H57	6.4514825980	5.6652341193	1.9873974240
C58	9.4950395957	7.3920206458	1.9266799505
H59	9.1920645518	8.1267298438	1.1745679641
H60	10.5439710912	7.1541952655	1.7380402383
H61	9.4315503809	7.8849710995	2.9010615251

Table 18 Fc

E = -510.61506621971 H, G = -510.479699 H, E(sl) = -510.62134555655 H

Fe1	0.0000000000	0.0000000000	0.0000000000
C2	-0.3748691947	1.1537287490	1.6853684839
C3	0.9814202930	0.7130435807	1.6853684839
C4	0.9814202930	-0.7130435807	1.6853684839
C5	-0.3748691947	-1.1537287490	1.6853684839
C6	-1.2131021966	-0.0000000000	1.6853684839
H7	1.8551560114	1.3478497384	1.6501140599
H8	1.8551560114	-1.3478497384	1.6501140599
H9	-0.7086065419	-2.1808666884	1.6501140599
H10	-2.2930989390	-0.0000000000	1.6501140599
H11	-0.7086065419	2.1808666884	1.6501140599
C12	-1.2131021966	-0.0000000000	-1.6853684839
C13	-0.3748691947	-1.1537287490	-1.6853684839
C14	0.9814202930	-0.7130435807	-1.6853684839
C15	0.9814202930	0.7130435807	-1.6853684839
C16	-0.3748691947	1.1537287490	-1.6853684839
H17	-0.7086065419	-2.1808666884	-1.6501140599
H18	1.8551560114	-1.3478497384	-1.6501140599
H19	1.8551560114	1.3478497384	-1.6501140599
H20	-0.7086065419	2.1808666884	-1.6501140599
H21	-2.2930989390	-0.0000000000	-1.6501140599

Table 19 Fc^{+}

E = -510.38357879573 H, G = -510.239742 H, E(sl) = -510.42281996813

Fe1	-0.0004712633	-0.0020576387	0.0071898137
C2	-1.7564591920	-0.0521988493	-1.2137077013
C3	-1.7689759603	1.1416623123	-0.4443947619
C4	-1.7501051708	0.7828574635	0.9308690532
C5	-1.7306120271	-0.6412016601	1.0153782238
C6	-1.7363155966	-1.1575798213	-0.3155794415
H7	-1.7494275902	2.1486619951	-0.8368052745
H8	-1.7305523103	1.4704052336	1.7643801886
H9	-1.7100928205	-1.2237025659	1.9250448726
H10	-1.7124796891	-2.2012479776	-0.5943741222
H11	-1.7370350867	-0.1096523561	-2.2927735074
C12	1.7533009048	-0.0809737916	1.2101975214
C13	1.7186818955	1.1199089917	0.4410934741
C14	1.7235660160	0.7546283404	-0.9391826667
C15	1.7637568396	-0.6675037225	-1.0150501674
C16	1.7844690141	-1.1797508849	0.3092509805
H17	1.6882967583	2.1259145941	0.8339930336
H18	1.6933854055	1.4341977286	-1.7786860744
H19	1.7492195917	-1.2559980496	-1.9214360473
H20	1.7797014137	-2.2253143176	0.5834259864
H21	1.7395808127	-0.1463269537	2.2887974528

Table 20 Cc

E = -532.23690518171 H, G = -532.109047 H, E(sl) = -532.2434423008 H

Co1	-0.0041742204	-0.0011638238	0.0010145979
C2	-0.3618656241	1.1641706612	1.7939111210
C3	0.9735107141	0.7154933683	1.7721232306
C4	0.9658179136	-0.7268731453	1.7761251636
C5	-0.3735412301	-1.1624988499	1.8062614410
C6	-1.1987130557	0.0042155116	1.7374293034
H7	1.8573846601	1.3372136100	1.7477229956
H8	1.8429519872	-1.3582519806	1.7561582379
H9	-0.7168868965	-2.1864900698	1.7991479076
H10	-2.2794907790	0.0091982395	1.7029250732
H11	-0.6964402105	2.1909778675	1.7812996340
C12	-1.1970867750	-0.0043667243	-1.7339522388
C13	-0.3607102890	-1.1628622031	-1.8005344921
C14	0.9746494810	-0.7137099372	-1.7755621166
C15	0.9677154534	0.7285347445	-1.7786367954
C16	-0.3711968623	1.1631855536	-1.8015971383
H17	-0.6949157052	-2.1898608604	-1.7897292949
H18	1.8580895443	-1.3362236947	-1.7551398891
H19	1.8448433861	1.3598607208	-1.7592885223
H20	-0.7148276995	2.1871106102	-1.7899484154
H21	-2.2778437442	-0.0084540888	-1.6996997000

Table 21 Cc^{+}

E = -532.03253329334 H, G = -531.897786 H, E(sl) = -532.10568166213 H

Co1	-0.0011575799	-0.0010966513	0.0001939709
C2	-0.3683671402	1.1559387419	1.6768097039
C3	0.9863714104	0.7082035328	1.6773713873
C4	0.9788589654	-0.7174466748	1.6803474411
C5	-0.3804649427	-1.1506921317	1.6809758014
C6	-1.2134535503	0.0070362381	1.6767428550
H7	1.8625678843	1.3396517801	1.6540412678
H8	1.8483315808	-1.3582616237	1.6600800478
H9	-0.7183990238	-2.1762741849	1.6481826291
H10	-2.2936219680	0.0125274325	1.6660281416
H11	-0.6956016201	2.1848618854	1.6411700193
C12	-1.2135165981	-0.0059661957	-1.6756754453
C13	-0.3684358316	-1.1548754569	-1.6803563980
C14	0.9861309818	-0.7073479214	-1.6799939641
C15	0.9786554622	0.7183580012	-1.6788014992
C16	-0.3805773205	1.1518160372	-1.6782359909
H17	-0.6957132672	-2.1838769663	-1.6464633390
H18	1.8623756580	-1.3388663275	-1.6598823521
H19	1.8481000862	1.3591296740	-1.6566126627
H20	-0.7186009350	2.1772564193	-1.6426545191
H21	-2.2936807929	-0.0118426568	-1.6655145327

Gaussian calculated (UB3LYP/6-311+G, SDD on Fe, Co, Re)**

Table 22 [$Re(CO)_3$(dippf)Br], from Fe(III) XRD
E = -4656.57254763 H, G = -4656.075718 H, E(sl) = -4656.583566 H

Re1	-1.4610000000000	0.6280000000000	0.1140000000000
Br2	-0.4780000000000	0.3430000000000	2.6270000000000
P3	0.7790000000000	1.7270000000000	-0.6260000000000
Fe4	2.8240000000000	-1.0450000000000	0.2220000000000
P5	-0.6490000000000	-1.8400000000000	-0.3960000000000
O6	-2.8930000000000	1.1550000000000	-2.5660000000000
C7	0.0650000000000	3.0880000000000	-3.0430000000000
H8	0.2470000000000	3.2010000000000	-4.1190000000000
H9	0.2260000000000	4.0660000000000	-2.5810000000000
H10	-0.9870000000000	2.8210000000000	-2.9180000000000
C11	0.8520000000000	0.7080000000000	-3.3000000000000
H12	1.1350000000000	0.8960000000000	-4.3430000000000
H13	-0.1850000000000	0.3630000000000	-3.2970000000000
H14	1.4820000000000	-0.1020000000000	-2.9220000000000
C15	-0.4290000000000	-3.9970000000000	-2.3330000000000
H16	-0.1760000000000	-4.2250000000000	-3.3760000000000
H17	-1.3330000000000	-4.5640000000000	-2.0920000000000
H18	0.3820000000000	-4.3720000000000	-1.7060000000000
C19	-2.3050000000000	0.9170000000000	-1.5830000000000
C20	1.0040000000000	2.0010000000000	-2.4860000000000
H21	2.0360000000000	2.3520000000000	-2.5950000000000
C22	1.0150000000000	3.4970000000000	0.0290000000000
H23	0.1200000000000	4.0170000000000	-0.3350000000000
C24	-2.0520000000000	2.4070000000000	0.6560000000000
O25	-2.4500000000000	3.4490000000000	0.9700000000000
C26	-3.1440000000000	-0.0550000000000	0.8420000000000
O27	-4.1650000000000	-0.3720000000000	1.2890000000000
C28	2.3690000000000	0.9450000000000	-0.1540000000000
C29	1.6510000000000	-2.2910000000000	1.3720000000000
H30	1.1540000000000	-1.9290000000000	2.2600000000000
C31	1.1080000000000	-2.2340000000000	0.0400000000000
C32	-0.6590000000000	-2.4770000000000	-2.1960000000000
H33	0.2090000000000	-1.9670000000000	-2.6260000000000
C34	-1.8750000000000	-2.0620000000000	-3.0440000000000
H35	-1.9690000000000	-0.9830000000000	-3.1510000000000
H36	-2.8190000000000	-2.4380000000000	-2.6410000000000
H37	-1.7610000000000	-2.4830000000000	-4.0510000000000
C38	-1.5700000000000	-3.2390000000000	0.5210000000000
H39	-0.9810000000000	-4.1340000000000	0.2810000000000
C40	-1.5970000000000	-3.0940000000000	2.0500000000000
H41	-2.1310000000000	-3.9560000000000	2.4700000000000
H42	-2.1110000000000	-2.1870000000000	2.3730000000000
H43	-0.5970000000000	-3.0830000000000	2.4870000000000
C44	-3.0020000000000	-3.4540000000000	-0.0020000000000
H45	-3.4610000000000	-4.2770000000000	0.5600000000000

H46	-3.0380000000000	-3.7250000000000	-1.0580000000000
H47	-3.6330000000000	-2.5740000000000	0.1470000000000
C48	2.1530000000000	-2.6880000000000	-0.8460000000000
H49	2.1000000000000	-2.7540000000000	-1.9230000000000
C50	3.2920000000000	-3.0450000000000	-0.0670000000000
H51	4.2380000000000	-3.4000000000000	-0.4560000000000
C52	2.9790000000000	-2.8030000000000	1.3020000000000
H53	3.6510000000000	-2.9300000000000	2.1420000000000
C54	3.4410000000000	0.5130000000000	-1.0140000000000
H55	3.4340000000000	0.5050000000000	-2.0950000000000
C56	4.5270000000000	0.0800000000000	-0.2000000000000
H57	5.4610000000000	-0.3310000000000	-0.5600000000000
C58	4.1470000000000	0.2430000000000	1.1650000000000
H59	4.7400000000000	-0.0330000000000	2.0270000000000
C60	2.8220000000000	0.7630000000000	1.2000000000000
H61	2.2240000000000	0.9340000000000	2.0840000000000
C62	1.0220000000000	3.6000000000000	1.5640000000000
H63	0.9000000000000	4.6530000000000	1.8470000000000
H64	1.9770000000000	3.2600000000000	1.9740000000000
H65	0.2300000000000	3.0220000000000	2.0440000000000
C66	2.2630000000000	4.1990000000000	-0.5340000000000
H67	2.3350000000000	5.2040000000000	-0.1020000000000
H68	2.2460000000000	4.3120000000000	-1.6220000000000
H69	3.1750000000000	3.6570000000000	-0.2610000000000

Table 23 $[Re(CO)_3(dippf)Br]^+$, from XRD

E = -4656.34788093 H, G = -4655.851305 H, E(sl) = -4656.40945426 H

Re1	-1.0850000000000	-1.1090000000000	-0.1650000000000
Br2	-0.1780000000000	-0.3370000000000	-2.5900000000000
P3	1.3770000000000	-1.3800000000000	0.6580000000000
Fe4	2.2060000000000	2.0340000000000	-0.2010000000000
P5	-1.3810000000000	1.4480000000000	0.4340000000000
O6	-2.2840000000000	-2.2360000000000	2.4480000000000
C7	1.1830000000000	-2.8910000000000	3.0640000000000
H8	1.4170000000000	-2.9480000000000	4.1340000000000
H9	1.6610000000000	-3.7470000000000	2.5820000000000
H10	0.1000000000000	-3.0010000000000	2.9630000000000
C11	1.0490000000000	-0.3920000000000	3.3290000000000
H12	1.3620000000000	-0.4720000000000	4.3760000000000
H13	-0.0420000000000	-0.4500000000000	3.3070000000000
H14	1.3420000000000	0.6010000000000	2.9730000000000
C15	-1.9910000000000	3.4820000000000	2.4150000000000
H16	-1.8580000000000	3.7650000000000	3.4660000000000
H17	-3.0410000000000	3.6590000000000	2.1670000000000
H18	-1.3880000000000	4.1650000000000	1.8110000000000
C19	-1.8110000000000	-1.7660000000000	1.4920000000000
C20	1.6760000000000	-1.5370000000000	2.5190000000000
H21	2.7650000000000	-1.4950000000000	2.6440000000000
C22	2.2600000000000	-2.9220000000000	-0.0220000000000
H23	1.5900000000000	-3.7280000000000	0.3040000000000
C24	-0.9540000000000	-2.9620000000000	-0.7840000000000
O25	-0.9260000000000	-4.0570000000000	-1.1480000000000
C26	-2.8800000000000	-1.1110000000000	-0.9540000000000
O27	-3.9230000000000	-1.1990000000000	-1.4410000000000
C28	2.6010000000000	-0.0700000000000	0.1820000000000
C29	0.5540000000000	2.8270000000000	-1.3140000000000
H30	0.2110000000000	2.3380000000000	-2.2150000000000
C31	0.0770000000000	2.5360000000000	0.0050000000000
C32	-1.6130000000000	1.9960000000000	2.2460000000000
H33	-0.6120000000000	1.8430000000000	2.6690000000000
C34	-2.5700000000000	1.1160000000000	3.0690000000000
H35	-2.2520000000000	0.0760000000000	3.1210000000000
H36	-3.5930000000000	1.1310000000000	2.6870000000000
H37	-2.6010000000000	1.5010000000000	4.0950000000000
C38	-2.7670000000000	2.3950000000000	-0.4800000000000
H39	-2.5910000000000	3.4440000000000	-0.2090000000000
C40	-2.7250000000000	2.2870000000000	-2.0120000000000
H41	-3.5770000000000	2.8460000000000	-2.4170000000000
H42	-2.8030000000000	1.2560000000000	-2.3640000000000
H43	-1.8230000000000	2.7230000000000	-2.4460000000000
C44	-4.1630000000000	1.9980000000000	0.0380000000000
H45	-4.9120000000000	2.5740000000000	-0.5180000000000
H46	-4.3080000000000	2.2220000000000	1.0960000000000
H47	-4.3850000000000	0.9410000000000	-0.1250000000000

C48	0.9160000000000	3.2810000000000	0.9060000000000
H49	0.8550000000000	3.2800000000000	1.9850000000000
C50	1.8540000000000	4.0500000000000	0.1480000000000
H51	2.6000000000000	4.7210000000000	0.5530000000000
C52	1.6260000000000	3.7630000000000	-1.2320000000000
H53	2.1800000000000	4.1640000000000	-2.0720000000000
C54	3.3880000000000	0.7750000000000	1.0340000000000
H55	3.3690000000000	0.7860000000000	2.1150000000000
C56	4.2070000000000	1.6180000000000	0.2230000000000
H57	4.9080000000000	2.3600000000000	0.5830000000000
C58	3.9310000000000	1.3030000000000	-1.1440000000000
H59	4.3740000000000	1.7730000000000	-2.0130000000000
C60	2.9430000000000	0.2770000000000	-1.1660000000000
H61	2.4560000000000	-0.1170000000000	-2.0480000000000
C62	2.3430000000000	-2.9710000000000	-1.5580000000000
H63	2.5550000000000	-4.0010000000000	-1.8650000000000
H64	3.1680000000000	-2.3520000000000	-1.9260000000000
H65	1.4290000000000	-2.6500000000000	-2.0600000000000
C66	3.6540000000000	-3.1600000000000	0.5820000000000
H67	4.0720000000000	-4.0790000000000	0.1550000000000
H68	3.6470000000000	-3.2830000000000	1.6680000000000
H69	4.3440000000000	-2.3460000000000	0.3320000000000

Table 24 [$Re(CO)_3$(dippc)Br], from Fe(III) XRD

E = -4681.61684741 H, G = -4681.129527 H, E(sl) = -4681.62854808 H

Re1	-1.3610000000000	-0.8130000000000	-0.1250000000000
Br2	-0.4190000000000	-0.3560000000000	-2.6330000000000
P3	1.0120000000000	-1.6530000000000	0.6170000000000
Co4	2.6820000000000	1.4100000000000	-0.2090000000000
P5	-0.9150000000000	1.7730000000000	0.4000000000000
O6	-2.7050000000000	-1.5630000000000	2.5400000000000
C7	0.4630000000000	-3.0790000000000	3.0400000000000
H8	0.6800000000000	-3.1770000000000	4.1080000000000
H9	0.7220000000000	-4.0270000000000	2.5680000000000
H10	-0.6130000000000	-2.9320000000000	2.9410000000000
C11	0.9620000000000	-0.6240000000000	3.2870000000000
H12	1.2740000000000	-0.7740000000000	4.3260000000000
H13	-0.1060000000000	-0.4070000000000	3.2960000000000
H14	1.4870000000000	0.2530000000000	2.9060000000000
C15	-1.0200000000000	3.9070000000000	2.3660000000000
H16	-0.8200000000000	4.1520000000000	3.4150000000000
H17	-1.9880000000000	4.3450000000000	2.1160000000000
H18	-0.2600000000000	4.4000000000000	1.7610000000000
C19	-2.1580000000000	-1.2360000000000	1.5680000000000
C20	1.2610000000000	-1.8910000000000	2.4760000000000
H21	2.3260000000000	-2.1190000000000	2.5770000000000
C22	1.4310000000000	-3.3840000000000	-0.0380000000000
H23	0.5950000000000	-3.9920000000000	0.3210000000000
C24	-1.7290000000000	-2.6470000000000	-0.6790000000000
O25	-2.0070000000000	-3.7160000000000	-0.9980000000000
C26	-3.1310000000000	-0.3650000000000	-0.8310000000000
O27	-4.1860000000000	-0.2000000000000	-1.2590000000000
C28	2.5070000000000	-0.7110000000000	0.1500000000000
C29	1.3290000000000	2.5620000000000	-1.3210000000000
H30	0.8950000000000	2.1770000000000	-2.2290000000000
C31	0.7530000000000	2.4380000000000	-0.0120000000000
C32	-1.0340000000000	2.3740000000000	2.2050000000000
H33	-0.1080000000000	1.9820000000000	2.6330000000000
C34	-2.1850000000000	1.7740000000000	3.0270000000000
H35	-2.1220000000000	0.6940000000000	3.1130000000000
H36	-3.1670000000000	2.0170000000000	2.6200000000000
H37	-2.1440000000000	2.1860000000000	4.0410000000000
C38	-2.0340000000000	3.0180000000000	-0.5140000000000
H39	-1.5750000000000	3.9810000000000	-0.2690000000000
C40	-2.0320000000000	2.8780000000000	-2.0420000000000
H41	-2.6490000000000	3.6790000000000	-2.4620000000000
H42	-2.4460000000000	1.9260000000000	-2.3740000000000
H43	-1.0370000000000	2.9720000000000	-2.4720000000000
C44	-3.4800000000000	3.0280000000000	0.0080000000000
H45	-4.0580000000000	3.7510000000000	-0.5760000000000
H46	-3.5540000000000	3.3270000000000	1.0530000000000
H47	-3.9720000000000	2.0620000000000	-0.1050000000000

C48	1.7370000000000	2.9590000000000	0.8850000000000
H49	1.6730000000000	2.9900000000000	1.9600000000000
C50	2.8200000000000	3.5240000000000	0.1280000000000
H51	3.6900000000000	4.0070000000000	0.5460000000000
C52	2.5560000000000	3.2970000000000	-1.2340000000000
H53	3.1910000000000	3.5590000000000	-2.0670000000000
C54	3.5060000000000	-0.1360000000000	0.9930000000000
H55	3.5130000000000	-0.1370000000000	2.0720000000000
C56	4.5660000000000	0.3880000000000	0.1770000000000
H57	5.4570000000000	0.8730000000000	0.5460000000000
C58	4.2070000000000	0.2000000000000	-1.1670000000000
H59	4.7660000000000	0.5200000000000	-2.0330000000000
C60	2.9110000000000	-0.4130000000000	-1.1940000000000
H61	2.3400000000000	-0.6410000000000	-2.0790000000000
C62	1.4510000000000	-3.4730000000000	-1.5720000000000
H63	1.4650000000000	-4.5270000000000	-1.8640000000000
H64	2.3540000000000	-3.0100000000000	-1.9760000000000
H65	0.5940000000000	-3.0000000000000	-2.0480000000000
C66	2.7440000000000	-3.9560000000000	0.5220000000000
H67	2.9050000000000	-4.9540000000000	0.1040000000000
H68	2.7500000000000	-4.0540000000000	1.6090000000000
H69	3.5970000000000	-3.3370000000000	0.2310000000000

Table 25 $[Re(CO)_3(dippc)Br]^+$, from XRD

E = -4681.40763036 H, G = -4680.915209 H, E(sl) = -4681.47111759 H

Re1	1.4280000000000	-0.6960000000000	-0.1420000000000
Br2	0.3780000000000	-0.3030000000000	-2.6170000000000
Co3	-2.7470000000000	1.1710000000000	-0.2130000000000
P4	-0.8140000000000	-1.7240000000000	0.6490000000000
C5	-2.3800000000000	-0.8470000000000	0.1820000000000
P6	0.7820000000000	1.8040000000000	0.4290000000000
C7	-2.8290000000000	-0.6460000000000	-1.1680000000000
H8	-2.2420000000000	-0.8500000000000	-2.0500000000000
C9	-4.1220000000000	-0.0530000000000	-1.1370000000000
H10	-4.7050000000000	0.2380000000000	-1.9980000000000
C11	-4.4850000000000	0.1440000000000	0.2270000000000
H12	-5.3920000000000	0.6060000000000	0.5870000000000
C13	-3.4180000000000	-0.3410000000000	1.0360000000000
H14	-3.3990000000000	-0.3110000000000	2.1130000000000
C15	-0.9690000000000	2.2880000000000	-0.0180000000000
C16	-2.0020000000000	2.7650000000000	0.8630000000000
H17	-1.9540000000000	2.8080000000000	1.9390000000000
C18	-3.1270000000000	3.1690000000000	0.0880000000000
H19	-4.0570000000000	3.5570000000000	0.4770000000000
C20	-2.8200000000000	2.9250000000000	-1.2810000000000
H21	-3.4790000000000	3.0880000000000	-2.1210000000000
C22	-1.5100000000000	2.3670000000000	-1.3460000000000
H23	-1.0250000000000	1.9870000000000	-2.2320000000000
C24	-1.0640000000000	-1.9930000000000	2.5030000000000
H25	-2.1110000000000	-2.2940000000000	2.6050000000000
C26	-0.1850000000000	-3.1380000000000	3.0390000000000
H27	0.8780000000000	-2.9240000000000	2.9290000000000
H28	-0.3930000000000	-4.0950000000000	2.5610000000000
H29	-0.3810000000000	-3.2610000000000	4.1070000000000
C30	-0.8390000000000	-0.7250000000000	3.3350000000000
H31	-1.1240000000000	-0.9160000000000	4.3730000000000
H32	-1.4250000000000	0.1270000000000	2.9850000000000
H33	0.2120000000000	-0.4350000000000	3.3330000000000
C34	-1.1900000000000	-3.4560000000000	-0.0380000000000
H35	-0.3220000000000	-4.0210000000000	0.3180000000000
C36	-1.2050000000000	-3.5480000000000	-1.5720000000000
H37	-1.1270000000000	-4.6000000000000	-1.8570000000000
H38	-0.3910000000000	-3.0090000000000	-2.0530000000000
H39	-2.1470000000000	-3.1760000000000	-1.9820000000000
C40	-2.4660000000000	-4.0940000000000	0.5330000000000
H41	-2.5710000000000	-5.1010000000000	0.1190000000000
H42	-3.3590000000000	-3.5340000000000	0.2420000000000
H43	-2.4600000000000	-4.1930000000000	1.6190000000000
C44	0.7920000000000	2.4190000000000	2.2320000000000
H45	-0.0970000000000	1.9350000000000	2.6460000000000
C46	0.6300000000000	3.9440000000000	2.3890000000000
H47	0.3930000000000	4.1680000000000	3.4340000000000

H48	-0.1610000000000	4.3750000000000	1.7740000000000
H49	1.5560000000000	4.4720000000000	2.1540000000000
C50	1.9830000000000	1.9320000000000	3.0730000000000
H51	1.8670000000000	2.3120000000000	4.0920000000000
H52	2.9400000000000	2.2970000000000	2.7010000000000
H53	2.0440000000000	0.8500000000000	3.1360000000000
C54	1.7380000000000	3.1780000000000	-0.4890000000000
H55	1.1960000000000	4.0920000000000	-0.2250000000000
C56	3.1770000000000	3.3070000000000	0.0410000000000
H57	3.6710000000000	4.1180000000000	-0.5010000000000
H58	3.7650000000000	2.4050000000000	-0.1290000000000
H59	3.2250000000000	3.5530000000000	1.1000000000000
C60	1.7520000000000	3.0560000000000	-2.0180000000000
H61	2.3300000000000	3.8930000000000	-2.4190000000000
H62	0.7590000000000	3.1130000000000	-2.4620000000000
H63	2.2180000000000	2.1330000000000	-2.3600000000000
O64	2.8810000000000	-1.3330000000000	2.4980000000000
C65	2.3020000000000	-1.0580000000000	1.5340000000000
O66	4.1530000000000	0.1820000000000	-1.3570000000000
C67	3.1400000000000	-0.0900000000000	-0.8980000000000
C68	1.9430000000000	-2.4930000000000	-0.7290000000000
O69	2.2850000000000	-3.5330000000000	-1.0690000000000

Table 26 dippf

E = -1666.94553466 H, G = -1666.479442 H, E(sl) = -1666.95095143 H

P1	3.4210000000000	-0.3220000000000	-0.8130000000000
Fe2	0.0650000000000	-0.0860000000000	0.3800000000000
P3	-3.3190000000000	0.4520000000000	-0.6300000000000
C4	5.6670000000000	-1.7010000000000	0.1990000000000
H5	6.0980000000000	-2.3400000000000	0.9770000000000
H6	6.3410000000000	-0.8540000000000	0.0630000000000
H7	5.6580000000000	-2.2780000000000	-0.7320000000000
C8	3.4150000000000	-2.5060000000000	0.9790000000000
H9	3.9010000000000	-3.0520000000000	1.7950000000000
H10	3.3250000000000	-3.1900000000000	0.1290000000000
H11	2.4090000000000	-2.2400000000000	1.3050000000000
C12	-4.9640000000000	-1.9540000000000	-0.3580000000000
H13	-5.4430000000000	-2.7840000000000	-0.8890000000000
H14	-5.7220000000000	-1.5070000000000	0.2920000000000
H15	-4.1790000000000	-2.3740000000000	0.2750000000000
C16	4.2470000000000	-1.2710000000000	0.6010000000000
H17	4.3190000000000	-0.6170000000000	1.4760000000000
C18	4.6380000000000	1.1150000000000	-1.0720000000000
H19	5.5510000000000	0.6010000000000	-1.3950000000000
C20	2.0400000000000	0.5570000000000	0.0360000000000
C21	-1.5550000000000	-1.0900000000000	1.2370000000000
H22	-2.0310000000000	-0.8240000000000	2.1680000000000
C23	-1.9210000000000	-0.6110000000000	-0.0640000000000
C24	-4.4010000000000	-0.9380000000000	-1.3590000000000
H25	-3.6700000000000	-1.4620000000000	-1.9850000000000
C26	-5.4830000000000	-0.3870000000000	-2.3010000000000
H27	-5.0590000000000	0.3070000000000	-3.0320000000000
H28	-6.2730000000000	0.1420000000000	-1.7620000000000
H29	-5.9570000000000	-1.2070000000000	-2.8500000000000
C30	-4.1630000000000	0.9150000000000	0.9980000000000
H31	-4.2620000000000	0.0160000000000	1.6140000000000
C32	-3.3140000000000	1.9460000000000	1.7590000000000
H33	-3.8000000000000	2.2040000000000	2.7070000000000
H34	-3.2110000000000	2.8690000000000	1.1790000000000
H35	-2.3130000000000	1.5770000000000	1.9820000000000
C36	-5.5650000000000	1.4910000000000	0.7430000000000
H37	-5.9910000000000	1.8620000000000	1.6810000000000
H38	-6.2570000000000	0.7490000000000	0.3420000000000
H39	-5.5280000000000	2.3310000000000	0.0430000000000
C40	-0.9990000000000	-1.2040000000000	-0.9920000000000
H41	-0.9790000000000	-1.0240000000000	-2.0570000000000
C42	-0.1030000000000	-2.0480000000000	-0.2770000000000
H43	0.7160000000000	-2.6050000000000	-0.7050000000000
C44	-0.4420000000000	-1.9700000000000	1.1050000000000
H45	0.0630000000000	-2.4720000000000	1.9170000000000
C46	1.7100000000000	0.6680000000000	1.4270000000000
H47	2.2130000000000	0.1660000000000	2.2390000000000

C48	0.5920000000000	1.5410000000000	1.5660000000000
H49	0.1090000000000	1.8030000000000	2.4960000000000
C50	0.2120000000000	1.9800000000000	0.2650000000000
H51	-0.6200000000000	2.6230000000000	0.0240000000000
C52	1.0860000000000	1.3640000000000	-0.6750000000000
H53	1.0300000000000	1.4690000000000	-1.7480000000000
C54	4.1790000000000	1.9950000000000	-2.2450000000000
H55	4.9600000000000	2.7190000000000	-2.5020000000000
H56	3.2800000000000	2.5620000000000	-1.9900000000000
H57	3.9640000000000	1.4010000000000	-3.1370000000000
C58	4.9590000000000	1.9640000000000	0.1630000000000
H59	5.7000000000000	2.7320000000000	-0.0860000000000
H60	5.3690000000000	1.3700000000000	0.9830000000000
H61	4.0650000000000	2.4730000000000	0.5320000000000

Table 27 dippf^{+}

E = -1666.72919357 H, G = -1666.264193 H, E(sl) = -1666.78125565 H

P1	3.5910000000000	0.0640000000000	-0.7050000000000
Fe2	0.0600000000000	-0.1090000000000	0.0270000000000
P3	-3.4680000000000	0.5980000000000	0.1910000000000
C4	5.7790000000000	-1.6820000000000	-0.4140000000000
H5	6.1580000000000	-2.6470000000000	-0.0670000000000
H6	6.4480000000000	-0.9120000000000	-0.0250000000000
H7	5.8510000000000	-1.6760000000000	-1.5060000000000
C8	3.4910000000000	-2.7280000000000	-0.3470000000000
H9	3.9200000000000	-3.6320000000000	0.0950000000000
H10	3.4880000000000	-2.8590000000000	-1.4330000000000
H11	2.4530000000000	-2.6620000000000	-0.0130000000000
C12	-5.0450000000000	-0.5470000000000	-1.9800000000000
H13	-5.5470000000000	-0.3460000000000	-2.9310000000000
H14	-5.7760000000000	-1.0300000000000	-1.3280000000000
H15	-4.2430000000000	-1.2630000000000	-2.1770000000000
C16	4.3260000000000	-1.5010000000000	0.0560000000000
H17	4.3220000000000	-1.4050000000000	1.1460000000000
C18	4.8030000000000	1.4250000000000	-0.1750000000000
H19	5.7180000000000	1.0950000000000	-0.6770000000000
C20	2.1670000000000	0.4180000000000	0.4210000000000
C21	-1.4610000000000	-1.5800000000000	-0.2040000000000
H22	-1.8020000000000	-2.2400000000000	0.5780000000000
C23	-2.0550000000000	-0.3270000000000	-0.5600000000000
C24	-4.5210000000000	0.7640000000000	-1.3820000000000
H25	-3.7980000000000	1.1930000000000	-2.0870000000000
C26	-5.6300000000000	1.8120000000000	-1.1940000000000
H27	-5.2360000000000	2.7530000000000	-0.8050000000000
H28	-6.4130000000000	1.4690000000000	-0.5150000000000
H29	-6.1040000000000	2.0200000000000	-2.1580000000000
C30	-4.2700000000000	-0.7230000000000	1.2760000000000
H31	-4.2780000000000	-1.6720000000000	0.7310000000000
C32	-3.4610000000000	-0.8820000000000	2.5760000000000
H33	-3.9070000000000	-1.6640000000000	3.1970000000000
H34	-3.4710000000000	0.0460000000000	3.1540000000000
H35	-2.4180000000000	-1.1560000000000	2.4040000000000
C36	-5.7180000000000	-0.3400000000000	1.6220000000000
H37	-6.1210000000000	-1.0560000000000	2.3440000000000
H38	-6.3760000000000	-0.3490000000000	0.7530000000000
H39	-5.7720000000000	0.6520000000000	2.0810000000000
C40	-1.2490000000000	0.2040000000000	-1.6230000000000
H41	-1.3870000000000	1.1680000000000	-2.0910000000000
C42	-0.2300000000000	-0.7300000000000	-1.9570000000000
H43	0.5270000000000	-0.6010000000000	-2.7170000000000
C44	-0.3540000000000	-1.8370000000000	-1.0720000000000
H45	0.2700000000000	-2.7180000000000	-1.0590000000000
C46	1.5990000000000	-0.3630000000000	1.4770000000000
H47	1.9650000000000	-1.3180000000000	1.8210000000000

C48	0.4780000000000	0.3340000000000	2.0260000000000
H49	-0.1330000000000	0.0010000000000	2.8510000000000
C50	0.3210000000000	1.5450000000000	1.2950000000000
H51	-0.4540000000000	2.2830000000000	1.4420000000000
C52	1.3310000000000	1.5780000000000	0.2950000000000
H53	1.4400000000000	2.3480000000000	-0.4550000000000
C54	4.4230000000000	2.7830000000000	-0.7840000000000
H55	5.2490000000000	3.4880000000000	-0.6550000000000
H56	3.5530000000000	3.2230000000000	-0.2890000000000
H57	4.2130000000000	2.7100000000000	-1.8540000000000
C58	5.0760000000000	1.5330000000000	1.3290000000000
H59	5.8620000000000	2.2710000000000	1.5130000000000
H60	5.4100000000000	0.5880000000000	1.7640000000000
H61	4.1880000000000	1.8620000000000	1.8760000000000

Table 28 dippc

E = -1688.85525583 H, G = -1688.394204 H, E(sl) = -1688.86085304 H

P1	3.5010000000000	-0.3130000000000	-0.8360000000000
Co2	0.0680000000000	-0.0930000000000	0.4080000000000
P3	-3.3940000000000	0.4310000000000	-0.6500000000000
C4	5.7070000000000	-1.7790000000000	0.1370000000000
H5	6.1250000000000	-2.4400000000000	0.9040000000000
H6	6.4060000000000	-0.9510000000000	0.0040000000000
H7	5.6710000000000	-2.3440000000000	-0.8000000000000
C8	3.4340000000000	-2.5200000000000	0.9210000000000
H9	3.9030000000000	-3.0930000000000	1.7280000000000
H10	3.3200000000000	-3.1890000000000	0.0620000000000
H11	2.4360000000000	-2.2270000000000	1.2510000000000
C12	-5.1100000000000	-1.9170000000000	-0.3240000000000
H13	-5.5970000000000	-2.7550000000000	-0.8340000000000
H14	-5.8680000000000	-1.4330000000000	0.2970000000000
H15	-4.3430000000000	-2.3310000000000	0.3360000000000
C16	4.3050000000000	-1.3080000000000	0.5560000000000
H17	4.4040000000000	-0.6700000000000	1.4410000000000
C18	4.7550000000000	1.0960000000000	-1.0820000000000
H19	5.6480000000000	0.5710000000000	-1.4410000000000
C20	2.1510000000000	0.5810000000000	0.0330000000000
C21	-1.6860000000000	-1.0710000000000	1.2690000000000
H22	-2.1630000000000	-0.7760000000000	2.1910000000000
C23	-2.0370000000000	-0.6440000000000	-0.0290000000000
C24	-4.5080000000000	-0.9490000000000	-1.3490000000000
H25	-3.7850000000000	-1.5110000000000	-1.9510000000000
C26	-5.5640000000000	-0.3960000000000	-2.3190000000000
H27	-5.1120000000000	0.2610000000000	-3.0670000000000
H28	-6.3410000000000	0.1740000000000	-1.8050000000000
H29	-6.0580000000000	-1.2180000000000	-2.8470000000000
C30	-4.2300000000000	0.9830000000000	0.9530000000000
H31	-4.3490000000000	0.1160000000000	1.6110000000000
C32	-3.3520000000000	2.0280000000000	1.6620000000000
H33	-3.8230000000000	2.3400000000000	2.6000000000000
H34	-3.2330000000000	2.9200000000000	1.0390000000000
H35	-2.3560000000000	1.6480000000000	1.8930000000000
C36	-5.6180000000000	1.5800000000000	0.6750000000000
H37	-6.0370000000000	1.9960000000000	1.5970000000000
H38	-6.3260000000000	0.8380000000000	0.3010000000000
H39	-5.5620000000000	2.3920000000000	-0.0570000000000
C40	-1.0680000000000	-1.2460000000000	-0.9210000000000
H41	-1.0380000000000	-1.0990000000000	-1.9910000000000
C42	-0.2380000000000	-2.1400000000000	-0.1860000000000
H43	0.5590000000000	-2.7440000000000	-0.5920000000000
C44	-0.5650000000000	-1.9740000000000	1.1780000000000
H45	-0.0910000000000	-2.4640000000000	2.0160000000000
C46	1.8250000000000	0.6840000000000	1.4080000000000
H47	2.3340000000000	0.1890000000000	2.2220000000000

C48	0.7150000000000	1.5890000000000	1.5670000000000
H49	0.2670000000000	1.8700000000000	2.5090000000000
C50	0.3310000000000	2.0380000000000	0.2880000000000
H51	-0.4860000000000	2.7030000000000	0.0550000000000
C52	1.1470000000000	1.3460000000000	-0.6620000000000
H53	1.0710000000000	1.4430000000000	-1.7350000000000
C54	4.2860000000000	2.0210000000000	-2.2160000000000
H55	5.0700000000000	2.7440000000000	-2.4640000000000
H56	3.3980000000000	2.5890000000000	-1.9240000000000
H57	4.0460000000000	1.4590000000000	-3.1230000000000
C58	5.1220000000000	1.9010000000000	0.1690000000000
H59	5.8760000000000	2.6590000000000	-0.0730000000000
H60	5.5350000000000	1.2730000000000	0.9630000000000
H61	4.2480000000000	2.4190000000000	0.5730000000000

Table 29 dippc^{+}

E = -1688.66050061 H, G = -1688.19197 H, E(sl) = -1688.71322683 H

P1	3.3830000000000	-0.2270000000000	-0.8340000000000
Co2	0.0680000000000	-0.1650000000000	0.4760000000000
P3	-3.2790000000000	0.5430000000000	-0.4990000000000
C4	5.7460000000000	-1.5470000000000	-0.0750000000000
H5	6.2560000000000	-2.2170000000000	0.6230000000000
H6	6.3700000000000	-0.6590000000000	-0.1860000000000
H7	5.7000000000000	-2.0550000000000	-1.0430000000000
C8	3.5940000000000	-2.5220000000000	0.7920000000000
H9	4.1570000000000	-3.0960000000000	1.5340000000000
H10	3.4860000000000	-3.1510000000000	-0.0960000000000
H11	2.5980000000000	-2.3450000000000	1.2050000000000
C12	-4.8490000000000	-1.8620000000000	-1.0310000000000
H13	-5.2760000000000	-2.5040000000000	-1.8060000000000
H14	-5.6590000000000	-1.6010000000000	-0.3460000000000
H15	-4.1170000000000	-2.4570000000000	-0.4780000000000
C16	4.3400000000000	-1.2210000000000	0.4570000000000
H17	4.4450000000000	-0.6240000000000	1.3700000000000
C18	4.4850000000000	1.2920000000000	-1.1210000000000
H19	5.3830000000000	0.8260000000000	-1.5420000000000
C20	2.0370000000000	0.5480000000000	0.1790000000000
C21	-1.5550000000000	-1.2490000000000	1.1870000000000
H22	-2.0400000000000	-1.0850000000000	2.1360000000000
C23	-1.9200000000000	-0.6400000000000	-0.0600000000000
C24	-4.2190000000000	-0.6200000000000	-1.6740000000000
H25	-3.4170000000000	-0.9540000000000	-2.3420000000000
C26	-5.2180000000000	0.1650000000000	-2.5410000000000
H27	-4.7460000000000	1.0230000000000	-3.0250000000000
H28	-6.0700000000000	0.5320000000000	-1.9650000000000
H29	-5.6130000000000	-0.4870000000000	-3.3250000000000
C30	-4.2690000000000	0.6120000000000	1.1070000000000
H31	-4.3680000000000	-0.4020000000000	1.5090000000000
C32	-3.5420000000000	1.4990000000000	2.1340000000000
H33	-4.1080000000000	1.5240000000000	3.0690000000000
H34	-3.4620000000000	2.5280000000000	1.7700000000000
H35	-2.5350000000000	1.1480000000000	2.3700000000000
C36	-5.6750000000000	1.1780000000000	0.8500000000000
H37	-6.1920000000000	1.3190000000000	1.8040000000000
H38	-6.2900000000000	0.5160000000000	0.2410000000000
H39	-5.6300000000000	2.1530000000000	0.3550000000000
C40	-0.9630000000000	-1.1130000000000	-1.0260000000000
H41	-0.9180000000000	-0.8120000000000	-2.0620000000000
C42	-0.0690000000000	-2.0230000000000	-0.3960000000000
H43	0.7680000000000	-2.5160000000000	-0.8670000000000
C44	-0.4300000000000	-2.1000000000000	0.9790000000000
H45	0.0720000000000	-2.6800000000000	1.7400000000000
C46	1.7270000000000	0.4390000000000	1.5750000000000
H47	2.2510000000000	-0.1750000000000	2.2910000000000

C48	0.5990000000000	1.2600000000000	1.8700000000000
H49	0.1320000000000	1.3690000000000	2.8370000000000
C50	0.1800000000000	1.8790000000000	0.6580000000000
H51	-0.6750000000000	2.5270000000000	0.5330000000000
C52	1.0420000000000	1.4250000000000	-0.3800000000000
H53	0.9480000000000	1.6790000000000	-1.4240000000000
C54	3.8970000000000	2.1990000000000	-2.2130000000000
H55	4.6420000000000	2.9410000000000	-2.5150000000000
H56	3.0260000000000	2.7540000000000	-1.8550000000000
H57	3.6080000000000	1.6350000000000	-3.1030000000000
C58	4.8800000000000	2.0890000000000	0.1260000000000
H59	5.5810000000000	2.8840000000000	-0.1470000000000
H60	5.3700000000000	1.4720000000000	0.8820000000000
H61	4.0110000000000	2.5670000000000	0.5880000000000

Table 30 Fc

E = -511.107420031 H, G = -510.971401 H, E = -511.110735031 H

Fe1	-0.0000000000000	0.0010000000000	0.0000000000000
C2	-1.6880000000000	-0.3540000000000	1.1620000000000
C3	1.6880000000000	0.9960000000000	0.6950000000000
H4	1.6670000000000	1.8830000000000	1.3140000000000
C5	1.6870000000000	-0.3530000000000	1.1620000000000
C6	1.6860000000000	-1.2150000000000	0.0230000000000
H7	1.6620000000000	-2.2970000000000	0.0440000000000
C8	1.6860000000000	-0.3980000000000	-1.1480000000000
H9	1.6620000000000	-0.7520000000000	-2.1710000000000
C10	1.6880000000000	0.9690000000000	-0.7330000000000
H11	1.6650000000000	1.8320000000000	-1.3850000000000
C12	-1.6860000000000	-1.2150000000000	0.0230000000000
H13	-1.6620000000000	-2.2970000000000	0.0430000000000
C14	-1.6860000000000	-0.3970000000000	-1.1480000000000
H15	-1.6620000000000	-0.7510000000000	-2.1710000000000
C16	-1.6870000000000	0.9690000000000	-0.7330000000000
H17	-1.6650000000000	1.8330000000000	-1.3850000000000
C18	-1.6890000000000	0.9950000000000	0.6950000000000
H19	-1.6670000000000	1.8830000000000	1.3150000000000
H20	-1.6650000000000	-0.6690000000000	2.1970000000000
H21	1.6640000000000	-0.6680000000000	2.1970000000000

Table 31 Fc^+

E = -510.875392848 H, G = -510.742578 H, E(sl) = -510.938682798 H

Fe1	-0.0000000000000	-0.0010000000000	0.0030000000000
C2	1.7050000000000	-0.6270000000000	1.0380000000000
C3	1.7120000000000	0.7970000000000	0.9140000000000
C4	1.7690000000000	1.1140000000000	-0.4740000000000
C5	1.7980000000000	-0.1040000000000	-1.2040000000000
C6	1.7570000000000	-1.1790000000000	-0.2770000000000
H7	1.6860000000000	1.5070000000000	1.7270000000000
H8	1.7640000000000	2.1070000000000	-0.9000000000000
H9	1.8080000000000	-0.1960000000000	-2.2810000000000
H10	1.7490000000000	-2.2300000000000	-0.5260000000000
H11	1.6760000000000	-1.1860000000000	1.9610000000000
C12	-1.7980000000000	-0.1030000000000	-1.2040000000000
C13	-1.7690000000000	1.1140000000000	-0.4740000000000
C14	-1.7120000000000	0.7960000000000	0.9150000000000
C15	-1.7050000000000	-0.6280000000000	1.0380000000000
C16	-1.7570000000000	-1.1790000000000	-0.2770000000000
H17	-1.7640000000000	2.1070000000000	-0.8980000000000
H18	-1.6860000000000	1.5060000000000	1.7280000000000
H19	-1.6770000000000	-1.1880000000000	1.9600000000000
H20	-1.7490000000000	-2.2290000000000	-0.5280000000000
H21	-1.8080000000000	-0.1940000000000	-2.2810000000000

Table 32 Cc

E = -533.014233691 H, G = -532.886686 H, E(sl) = -533.017708663 H

Co1	-0.0000000000000	0.0070000000000	0.0000000000000
C2	-1.7910000000000	-0.9940000000000	0.7020000000000
C3	1.7490000000000	0.3770000000000	1.1410000000000
H4	1.7320000000000	0.7040000000000	2.1700000000000
C5	1.7910000000000	-0.9940000000000	0.7020000000000
C6	1.7910000000000	-0.9940000000000	-0.7030000000000
H7	1.7780000000000	-1.8610000000000	-1.3450000000000
C8	1.7490000000000	0.3770000000000	-1.1400000000000
H9	1.7330000000000	0.7050000000000	-2.1700000000000
C10	1.8090000000000	1.2190000000000	0.0000000000000
H11	1.7980000000000	2.2980000000000	0.0010000000000
C12	-1.7910000000000	-0.9940000000000	-0.7020000000000
H13	-1.7780000000000	-1.8610000000000	-1.3450000000000
C14	-1.7490000000000	0.3770000000000	-1.1400000000000
H15	-1.7330000000000	0.7050000000000	-2.1700000000000
C16	-1.8090000000000	1.2190000000000	0.0000000000000
H17	-1.7980000000000	2.2980000000000	0.0010000000000
C18	-1.7490000000000	0.3770000000000	1.1410000000000
H19	-1.7320000000000	0.7040000000000	2.1700000000000
H20	-1.7780000000000	-1.8620000000000	1.3440000000000
H21	1.7780000000000	-1.8620000000000	1.3440000000000

Table 33 Cc^{+}

E = -532.807975315 H, G = -532.673169 H, E(sl) = -532.87151282 H

Co1	-0.0000000000000	0.0010000000000	-0.0000000000000
C2	-1.6730000000000	-0.8630000000000	0.8520000000000
C3	1.6740000000000	0.7050000000000	0.9870000000000
H4	1.6500000000000	1.3310000000000	1.8660000000000
C5	1.6740000000000	-0.7220000000000	0.9750000000000
C6	1.6740000000000	-1.1510000000000	-0.3840000000000
H7	1.6490000000000	-2.1740000000000	-0.7280000000000
C8	1.6740000000000	0.0100000000000	-1.2120000000000
H9	1.6500000000000	0.0180000000000	-2.2920000000000
C10	1.6750000000000	1.1570000000000	-0.3650000000000
H11	1.6510000000000	2.1860000000000	-0.6900000000000
C12	-1.6730000000000	-1.0780000000000	-0.5570000000000
H13	-1.6490000000000	-2.0360000000000	-1.0530000000000
C14	-1.6740000000000	0.1970000000000	-1.1970000000000
H15	-1.6490000000000	0.3730000000000	-2.2620000000000
C16	-1.6750000000000	1.1990000000000	-0.1820000000000
H17	-1.6510000000000	2.2660000000000	-0.3430000000000
C18	-1.6750000000000	0.5430000000000	1.0840000000000
H19	-1.6510000000000	1.0280000000000	2.0490000000000
H20	-1.6480000000000	-1.6320000000000	1.6100000000000
H21	1.6490000000000	-1.3640000000000	1.8420000000000